MULTISCALE MODELING AND UNCERTAINTY QUANTIFICATION OF COMPOSITE MATERIALS IN HIGH STRAIN RATE APPLICATION

By

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To my parents
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Failure simulation of composite materials is a challenging task due to various failure modes as well as the statistical nature of manufacturing defects, which are much larger than that of metallic materials. Although it might be premature to develop a general purpose numerical algorithm to predict failure of composite materials, it is possible if the focus is limited to a specific application, such as high strain rate impact phenomenon. Due to a short time period of impact, there is no need to consider cyclic loading and unloading scenarios. It is possible to model the material behavior under the monotonic loading condition. Under such a simplification, fiber breakage is considered as the major failure mode and all other progressive failure modes can be effectively ignored. Strain rate dependency of the mechanical properties of both fiber and matrix is also considered as an important factor under impact loading.

A key contribution of the current research is to utilize the surrogate modeling technique to connect between different scales. In the lowest scale, the stiffness and strength of individual fiber are measured and represented as a statistical distribution. Then, the stiffness and failure strength of prepreg are modeled using a surrogate model,
whose input variables are the volume fraction, stiffness and strength of fibers. The surrogate model is constructed by sampling input space and calculating the stiffness and strength of prepreg using analytical and numerical calculations. In the highest scale, the stiffness and strength of composite plate are modeled again using a surrogate model. In this scale, the surrogate-based material model is implemented into a commercial software to simulate the strength of composite plate.

One of the biggest challenges in designing composites structures is the considerable uncertainties in their mechanical properties. The uncertainties come from inherent variation in mechanical properties of the constituents and the unavoidable manufacturing imperfection. In metallic structures, such as airplane frame made of aluminum, the variability in the material properties is estimated using dozens of coupon tests, while the error in design and manufacturing is detected by a handful of element tests. However, in the case of composite material, the variability and design error are estimated simultaneously at the element or component level, which requires much more number of tests. The second contribution of the current research is to estimate the uncertainty in composite structure using a similar number of tests as in the metallic structures. In order to achieve this, uncertainty in the lower scale is propagated to the upper scale using surrogate modeling, and Bayesian inference is used to reduce epistemic uncertainty in the upper scale. The proposed framework was demonstrated using three-level scales: fibers in microscale, prepreg in mesoscale, and composite plates in macroscale. The results showed that the uncertainty with 29 fiber tests and 4 prepreg tests are more accurate than the uncertainty of 18 prepreg tests.
CHAPTER 1
INTRODUCTION

1.1 Multiscale Modeling of Composite Materials

Composite materials are gaining increasing prominence in engineering applications. They allow to take advantage of different properties of component materials, of the layup configuration and of the interaction between the constituents to obtain a tailored behavior. Composite materials may present high stiffness and damping, improved strength and toughness, improved thermal conductivity and electrical permittivity, improved permeability, and unusual physical properties such as negative Poisson’s ratio and negative stiffness inclusions [1].

For most of the analyses of composite structures, instead of taking the individual constituent elastic property and geometrical distribution into consideration, effective or homogenized stiffness and Poisson’s ratio are used. These effective properties are usually difficult or expensive to measure and in the design stage the composition may vary substantially, making frequent measurements prohibitive. A lot of effort has been put into the development of analytical and numerical approaches to derive effective properties.

1.1.1 Homogenization of Composite Materials

A variety of theories have been developed for homogenization of composite materials analytically, such as effective medium models of Eshelby [2], Hashin [3] and Mori and Tanaka [4]. Voigt [5] and Reuss [6] formulated rigorous bounds for the effective moduli of composites with prescribed volume fraction. If the microstructure is composed of a matrix and a spherical or spheroidal inclusions, the effective behavior of composites can be obtained by means of the self-consistent method [7-9]. Analytical
homogenization methods had been pioneered by Bensoussan [10] and Sanchez-Palencia [11]. The active computational approaches had been initiated by Guedes and Kikuchi [12]. Over the past decade major contributions have been made to extending the theory of computational homogenization to nonlinear regime [13-16] and to improving fidelity and computational efficiency of numerical simulations [17-21].

The Voigt upper bound on the effective elastic modulus, $M_v$, of a mixture of N material phases is

$$M_v = \sum_{i=1}^{N} f_i M_i$$  \hspace{1cm} (1-1)

where $f_i$ is the volume fraction of the $i^{th}$ constituent and $M_i$ the elastic modulus of the $i^{th}$ constituent. The Voigt upper bound is based on iso-strain assumption and is known as the rule of mixtures. Based on the rule of mixtures, the axial stiffness of unidirectional fiber reinforced composites is given as

$$E_i = f E_f + (1-f) E_m$$ \hspace{1cm} (1-2)

where $f$ is the volume fraction of the fibers, $E_f$ is the elastic stiffness of the fibers and $E_m$ is the elastic stiffness of the matrix. This is a good approximation since for unidirectional fiber reinforced composites under axial loading, the iso-strain assumption usually holds.

The Reuss lower bound of the effective elastic modulus, $M_R$, is

$$\frac{1}{M_R} = \sum_{i=1}^{N} \frac{f_i}{M_i}$$ \hspace{1cm} (1-3)

The Reuss lower bound is based on iso-stress assumption and is known as the inverse rule of mixtures. Based on the inverse rule of mixtures, the transverse stiffness of unidirectional fiber reinforced composites is given as
This is a poor approximation for $E_2$ because of the non-uniform distribution of stress and strain during transverse loading.

And the traditional numerical method is representative volume element (RVE). Such work can be found in Smit [22], Feyel [23], Miehe et al. [24], Terada and Kikuchi [17]. Renard et al. [25] first introduced the idea of using directly a finite element discretization of the microstructure, linked to the macroscopic scale, using homogenization rules. RVE is the smallest volume over which a measurement can be made to obtain a representative value of the whole. The popularity of RVE comes from the periodic characteristics of unidirectional fiber reinforced composites [26]. In the case of periodic materials, one can simply study the behavior of a periodic unit cell so that computational cost can be saved. RVE approach can be used to characterizing heterogeneous materials with macroscopically and statistically homogeneous structure [27, 28].

For unidirectional fiber reinforced composites, square packing and hexagonal packing are the most popular shapes of RVE [29-31]. The appropriate volume of a RVE need to meet two criteria [32]. First, it must be small enough with respect to the dimensions of the macro scale so that it can be considered as a material point. Second, it must be large enough with respect to the scale of the inclusion phase to have elastic properties independent of the loading condition [33].

1.1.2 Classification of Multiscale Procedures

Many engineering problems are solved at macroscopic scale with homogenized properties. However, when higher accuracy is required, we need to refer directly to the
microscopic scale. Then multi-scale modeling is needed to couple macroscopic and microscopic models to take advantage of the efficiency of macroscopic models and the accuracy of the microscopic models [34].

Most composite materials are multi-scale in nature, i.e. the scale of the constituents is of lower order than the scale of the structure [1]. The length scales range from the fiber size whose dimension is measured in microns, to the individual plies in laminates whose thicknesses are measured in fractions of millimeters, to the laminates themselves whose sizes are measured in millimeters, e.g. 30-40 mm. The laminates then form parts of composite structures whose sizes are measured in meters. The physical phenomena observed at any of these length scales are linked to those on the neighboring length scales.

For unidirectional fiber reinforced composites, the overall hierarchy of multi-scale analysis is composed of micro-level (fibers and matrix), meso-level (plies) and macro-level (laminated composites). Since all damage and failure modes initiate in the micro-level, damage and failure criteria are applied to micro-level stresses and strains. At the constituent level, damage and failure modes are simplified and physics-based and there are three potential modes: fiber breakage, matrix cracking and interfacial debonding. At the macro-level, more complicated damage modes exist. For example, interlaminar delamination, matrix cracking in a cross-ply laminar and fiber splitting in a longitudinal layer are some of the potential damage modes. All of these are associated with matrix cracking. Each of these may require a different criterion and failure strength. However, when using micro-level damage criteria, all of these can be described using the same
criterion associated with matrix cracking. As a result, damage and failure phenomena can be understood in unified and simplified concepts.

Currently there are two main approaches of multi-scale modeling [1]:

I. Sequential multi-scale procedures. In this approach, the micro-to-macro homogenization process is made separately from the structural analysis. Material response is defined through a set of constitutive equations. Parameters in these equations are subsequently identified with microscopic or macroscopic results, either true experiments or virtual experiments.

II. Integrated multi-scale procedures. This approach deals with all the complexity of local microstructures during all analyses, without summarizing it in some overall constitutive framework. In such cases, at each step of analysis, the actual response of each material point is calculated by calling for the micro-scale response, through the homogenization process. To some extent, through an averaging scheme, the internal variables in the overall boundary value problem are those of the micro-scale unit cells used in this multi-scale numerical procedure.

Both approaches estimate the constitutive relationship at a macroscopic point by performing micro-scale analysis.

1.2 Surrogate Modeling

A surrogate model is a model of an outcome of interest used when the outcome cannot be easily directly measured or calculated. Most engineering design problems require tests and/or simulations to evaluate objective function and constraints as function of design variables. However, tests or simulations of real world problems might
be quite expensive or take long time to complete. One simulation may take several minutes, hours, days or even weeks. As a result, design optimization and sensitivity analysis which require thousands or even millions of simulations become impossible. Surrogate modelling provides an approximation to the tests or simulations to alleviate the burden.

Due to the advantage, surrogate modeling technique has been used extensively in the design and optimization of computationally expensive problems. Barthelemy and Haftka [35] reviewed the application of surrogate modeling techniques in structural optimization. They discussed about local, medium-range and global approximations. They covered both function approximations and problem approximations. Sobieszczanski-Sobieski and Haftka reviewed [36] different surrogate modeling applications in multidisciplinary optimization. Queipo and Haftka [37] provided a comprehensive discussion of the fundamental issues in surrogate-based analysis and optimization. Key steps in surrogate modeling is discussed in detail, including design of experiment, numerical simulations at selected points, construction of surrogate model and model validation. There has been many successful applications of surrogate-based optimization, including rotor blade design and optimization [38], high speed civil transport [39], and injectors [40-42].

1.3 Bayesian Inference

Bayesian inference uses Bayes’ theorem to update the probability of a hypothesis as more evidence or information becomes available. Bayesian inference has found application in various discipline, such as science, engineering and medicine. In the field of engineering, Bayesian inference has been used in uncertainty quantification [43, 44]. Kim [45] and An [46] used Bayesian technique to incorporate the field failure
data into prior knowledge to obtain a more reliable prediction of fatigue life. There are also several studies using Bayesian inference to investigate the effect of tests on uncertainty reduction. Jiao [47] studied the effect of tests on structural safety using Bayesian inference. Tests can reduce uncertainty in the strength of a structure and help reduce probability of failure. An [48] investigated the effect of element tests on reducing uncertainty in element strength using Bayesian inference. Using Bayesian updating, the likelihood of unconservative estimation of element failure stress. Acar [49] proposed a methodology to investigate the effects of structural tests on aircraft safety. Bayesian updating is used to update the failure stress distribution based on element tests. Park [50] investigated the effect of the number of coupon and element tests on structural weight. Bayesian inference is used to reduce epistemic uncertainty using element test results.

1.4 Uncertainty Quantification of Composite Materials

Analysis of composite materials is challenging not only due to various failure modes but also because of large uncertainty. The uncertainties come from inherent variation in mechanical properties of the constituents and the unavoidable manufacturing imperfection, including variation in volume fractions of fiber and matrix, fiber misalignment, inadequate bonding between fibers and matrix, voids and porosity of the matrix, to list some of the important factors [51], [52], [53], [54] and [55]. Using a deterministic approach to design composite structures, we would be running the risk of underestimating/overestimating the material performance, which leads to either higher safety factors or premature failure [56]. And there is continued interest in uncertainty quantification, in developing rational design procedures for composites [57], [58], [59].
Uncertainty quantification of composites can be achieved using simulation or tests. A comprehensive approach of investigating all sources of uncertainty is too expensive or impractical to be performed. Simplifications have to be made to only consider the most important sources. Simulation results suffer from epistemic uncertainties which come from the simplifications as well as numerical errors. Due to limited budget, only a certain number of tests can be performed, thus test results suffer from sampling uncertainty [50]. We propose to combine simulation and test to perform uncertainty quantification to achieve higher accuracy and cost saving at the same time.

Most composite materials are multiscale in nature [1]. The scale of the constituents is of lower order than the scale of the structure. Uncertainty in upper scale is propagated from uncertainty in lower scale. In this research, we focus on the strength prediction of plain weave composites in high strain rate application. Three scales are investigated, including fiber scale or microscale (in micrometers), yarn and prepreg scale or mesoscale (in fraction of millimeters) and composites plate scale or macroscale (in dozens of millimeters), as shown in Figure 1-1. Tests are performed in all scales while simulations are performed in mesoscale and macroscale. In microscale and mesoscale, simulation and test are combined using Bayesian inference to effectively reduce both epistemic uncertainty of simulation and sampling uncertainty of test. Validation is performed in macroscale by comparing prediction against test data. Since we are focusing on strength prediction in high strain rate application and fiber is the major load-carrying component, we consider fiber breakage as the only failure mechanism and fiber properties and fiber volume fraction as the sources of uncertainty.
1.5 Objective

The main objective of this research is to build a framework of uncertainty quantification of multiscale modeling of composite materials. However, a thorough investigation of all sources of uncertainty for a general application is too complex and impractical. In order to make the uncertainty quantification feasible, we will focus on a specific application, i.e. high strain rate application. For this application, the problem is simplified because the loading condition is monotonic so that we don’t need to consider loading and unloading scenario. In such a loading condition, fiber breakage is the dominant failure mechanism. And the majority of the uncertainty in material performance would be propagated from constituents’ properties and volume fraction. From an engineering point of view, ignoring other factors would not lead to large error in our estimation and thus is acceptable. So in this research, the only sources of uncertainty that would be considered are fiber/matrix stiffness and strength and fiber volume fraction.

The other objective of this research is to develop a new framework of sequential multiscale modeling of composites. We choose sequential approach rather than integrated approach because the latter usually requires a huge amount of computational power and uncertainty quantification often needs numerous repetitions of response analysis. So using the integrated approach would make the uncertainty quantification impractical. Compared with traditional sequential approach which passes information from lower scale to higher scale through a limited number of parameters of a set of constitutive equations, we propose to bridge the scales using surrogate modeling technique which is more flexible and can pass more information to the next scale.
1.6 Outline

Chapter 2 introduces a multiscale framework of modeling composites in high strain rate application. Surrogate modeling technique is used to bridge the scales. Fiber breakage is considered as the major failure modes. Strain rate effect on mechanical properties of fiber and matrix is also considered as an important factor. The proposed framework is validated against test results and a built-in material model for composites in LS-DYNA.

Chapter 3 introduces a multiscale framework of uncertainty quantification of composites using Bayesian inference. Uncertainty in lower scale is propagated to upper scale through simulation. Tests are also performed in each scale. Simulation and test results are combined using Bayesian inference. At macroscale, open-hole tension tests are performed multiple times to provide statistical knowledge of tensile strength of composite plate with holes. The distribution of plate strength is also predicted using our proposed framework. Predicted distribution is compared with test results to validate our framework.

Finally, in Chapter 4 we present a summary and conclusions for this dissertation.
Figure 1-1. Multiple scales of composites. Photo courtesy of author.
CHAPTER 2
MULTISCALE MODELING OF COMPOSITES IN HIGH STRAIN RATE APPLICATION

In this section, a framework of multiscale modeling of unidirectional fiber reinforced composites is proposed and explained in detail. This framework utilizes surrogate modeling technique to bridge micro-scale model and macro-scale model. The details of micro-scale model and surrogate modeling are discussed. Fiber breakage is considered as the only failure mode. Strain rate effect is taken into consideration as an important factor.

2.1 Framework of Multiscale Modeling of Composites

A composite panel is composed of many laminates with different fiber orientations. And a laminate is composed of many fibers through the thickness. The main challenge in composite panel is that the failure occurs in micro-scale, while modeling occurs in macro-scale. A significant gap exists between the size of fracture initiation and the size of modeling interest, thus how to propagate information from micro scale to macro scale is a critical issue. This gap can be overcome by employing multi-scale modeling methods, which is often carried out using massive parallel processing [60]. As mentioned earlier, in this research, instead of massive parallel processing, we propose to use surrogate modeling to bridge microscale simulation and structural scale simulation to overcome the computational burden.

The basic idea of multi-scale modeling proposed in this research is illustrated in Figure 2-1, in which a composite panel is decomposed into three levels: composite panel, ply, and fiber-matrix cell. The basic requirement is that engineers model the composite panel in macro-scale, while the failure is determined in the micro-scale with fibers. In the composite panel level, the material behaves similar to anisotropic material.
In conventional macro-scale simulations, quite complicated failure models are used to represent complex failure phenomena [61]. However, complex failure models require more model parameters, and it is difficult to determine these parameters from experiments. In this scale, finite element analysis is often used to simulate the global response of composite panel, which requires calculating stresses at integration points of each element. The stresses at an integration point represent the averaged stresses around the point. It is possible that some fibers are broken and debonding may occur between a fiber and matrix. The macro-scale stress calculation should include all these effects in the averaged sense. Therefore, the multi-scale modeling is performed at each integration point of the FE mesh of the overall structure. Different finite element analysis programs take different ways on integration. For example, LS-DYNA uses a single point integration through the thickness of a layer, while Abaqus allows multiple integration points through the thickness of a composite panel. It would be the trade-off between accuracy and computational cost.

In the ply level, the stacking sequence of different directions of ply is considered in calculating the distribution of stress along the thickness direction. In the illustration in Figure 2-1, 10 plies with lay-up configuration [0/-45/90/45/0]s are used. The strain calculated in the panel level is converted to strain at each ply. In composite panel, it is assumed that the strain is composed of membrane and bending strains. Since the panel thickness is relatively small compared to the panel size, the traditional plate theory approximates that the strain varies linearly through the thickness. More specifically, the membrane strain is uniformly distributed through the thickness, while the bending strain varies linearly through the thickness. Therefore, using the superposition of uniform
membrane strain with linearly varying bending strain, it is possible to calculate strain at different locations in the ply.

The strain at different locations of a ply is then sent to fiber-matrix cell level to calculate stress at that location. Since the fiber direction changes at different plies, coordinate transformation must be performed to convert strains and resulting stresses between the local and global coordinate system. Also notice that delamination between plies initiates in this scale. However, this failure mode is not covered since the focus of current work is micro-scale modeling and propagating information in the micro-scale to macro-scale using surrogate modeling technique. In addition, under high strain rate application, the major failure modes are fiber breakage and fiber debonding, and all other failure modes can be secondary effects.

In the fiber-matrix level, fiber and matrix phases are modeled using different material properties. The interface between fiber and matrix is assumed to be perfect and no interfacial layer is considered. Two major failure modes, fiber fracture and fiber debonding, are considered. Fiber fracture is modeled using extended finite element method where cracks can be introduced without changing finite element mesh. In this scale, with six strain components sent from higher level, the plane stress RVE approach is used to calculate six components of averaged stresses, including the effect of fiber fracture and debonding. Instead of massive parallel processing, a surrogate is constructed for each stress component with six strain inputs generated from LHS sampling and stress outputs calculated from plane stress RVE model analyzed in Abaqus. The multi-scale surrogate modeling technique proposed here can overcome the computational burden in typical multi-scale modeling technique and provide
feasibility to uncertainty analysis based on large amount of repetition of response analysis in future research.

2.2 Plane Stress RVE Approach for Microscale Modeling

2.2.1 Plane Stress RVE

The traditional ways of calculating the material responses of micromechanical system are either analytical method or numerical method. The analytical methods ignore the interaction among fibers by assuming that fiber is relatively small [62]. This is not accurate since the nominal volume fraction of fiber is between 0.5 and 0.7, there exists a strong interaction between fibers. The traditional numerical method of micromechanical analysis of composites is using the representative volume element [63]. A typical RVE of unidirectional fiber-reinforced composites is shown in Figure 2-2. Assuming that the composite panel is composed of an infinite repetition of RVE, a single RVE is modeled with the periodic boundary condition. Once the diameter of the fiber is determined, the size of RVE is determined based on the volume fraction of fibers. It is noted that there are different types of RVE, which can be found in literature [31].

However, when it comes to uncertainty quantification, RVE becomes inappropriate since periodicity in RVE works against fiber fracture and uncertainty in the layout of fibers. For example, if the diameter of fiber is changed in RVE, it means the entire composite panel is made of fibers with the same diameter. Also, when the location of fiber is changed in the RVE, the entire fibers in the panel are periodically located, which is against the purpose of random distribution. Uncertainty is caused by randomly distributed distance between fibers, but the periodicity enforces the distance in a certain pattern.
In addition, the periodic boundary condition can often be inappropriate for composite plates. The dimensions in the membrane plane are large enough to be considered periodic, but the thickness direction of composite plates is relatively small, and the boundary effect becomes important in the response. In addition, most composite panels are under plane stress condition, and the free boundaries at the top and bottom surfaces do not follow periodic condition. Therefore, it is necessary to use different representative element. In this research, instead of RVE, plane stress RVE is used. The major different between RVE and plane stress RVE is the boundary condition. Plane stress RVE does not have periodic boundary condition in the thickness direction. As shown in Figure 2-3, plane stress RVE looks like a stack of several RVEs along the thickness direction. The idea is to apply the periodic boundary condition in membrane direction, same as the traditional RVE, but in the thickness direction, the actual behavior of a stack of fibers is simulated. However, it would be computationally too expensive to model the entire number of fibers throughout the thickness of composite panel, and it would violate the purpose of modeling a ‘representative’ behavior. On the other hand, if too small number of fibers are used, then the response of plane stress RVE is dominated by the boundary effect. In the following section, a study will be conducted to show how many fibers needs to be modeled in the stack of fibers in order to model the plane stress behavior of representative element, while preventing the effect of boundary at the top and bottom surfaces.

2.2.2 Size of Heterogeneous Structure

As discussed before, the plane stress RVE is composed of several RVEs in the thickness direction as shown in Figure 2-3. The appropriate size of the heterogeneous structure should be decided first because the material behavior of the element placed at
the most outer area would be different from the behavior of the one placed in the middle of the structure.

Figure 2-3 shows the deformed shape of the structures composed of several fibers in y direction and z direction under x direction displacement loading [64]. Only three fibers are modeled in y- and z-direction along with symmetric boundary condition. Jinuk Kim [64] found out that three RVEs in y direction and z direction should be enough for the size of the heterogeneous structure by comparing the effective stress in RVEs at different position. The averaged stress of the outer most fiber is about 27% different from the second layer fiber, but the difference between the second to the third layers is less than 1%. The difference in z-direction was much smaller than that of y-direction. Based on this observation, the heterogeneous structure model used in this research is shown in Figure 2-4. The mesh is composed of 29889 linear hexahedral elements of type C3D8 in Abaqus. Even if there are 3x3 layers of fibers, only the bottom corner layer fiber (highlighted cube) is used to calculate the averaged stress.

2.2.3 Boundary Conditions

The dimension in x direction is large enough to be considered periodic. And periodic boundary conditions will be imposed on the two surfaces perpendicular to x axis. The periodic boundary condition constrains the boundary to keep the relative displacement constant according to the strain on that boundary. It can be expressed as follows

\[ u_i (x_0 + d) = u_i (x_0) + \bar{\varepsilon}_{ij} d_j \]  

(2-1)

where \( \bar{\varepsilon}_{ij} \) is the averaged strain component and \( d \) is the characteristic distance. There is no applied force in plane stress RVE. Instead, the periodic boundary condition in Equation 2-1 is applied. From macro-scale composite panel analysis, six components of
strains at the current micro-scale fiber location are calculated. These strains are indeed the averaged strain components \( \bar{\varepsilon}_{ij} \) in Equation 2-1.

Concurrent multi-scale simulations start from a macro-scale simulation to calculate the averaged strain components at all integration points, and then micro-scale model is employed to calculate averaged stresses that include the effect of various failure modes. The objective of this research is to replace the concurrent micro-scale simulation with surrogate modeling.

For computational purpose, the periodic boundary condition cannot remove the rigid body motion. Therefore, in addition to the periodic boundary condition, minimum degrees-of-freedom (DOFs) need to be constrained so that the rigid body motion can be prevented.

### 2.2.4 Average Stress Values

The micro-scale simulation using plane stress RVE will calculate stress distribution in both fiber and matrix, which represents the micro-scale stress in heterogeneous medium. In order to utilize the micro-scale stresses into macro-scale simulation, it is necessary to scale up the micro-scale stresses to macro-scale stresses. The average scheme is used to calculate representative stress values of the plane stress RVE,

\[
\bar{\sigma}_{ij} = \frac{1}{V} \int_{V} \sigma_{ij} dV \tag{2-2}
\]

where \( \sigma_{ij} \) is the microscale stresses in the plane stress RVE, and \( V \) is the volume of the plane stress RVE.
As plane stress RVE itself is composed of lots of elements, the average can be achieved by integrating individual elements. In order to perform volume integral of each element, the Gaussian integration method is applied

$$\bar{\sigma}_{ij} = \frac{1}{V} \sum_{k=1}^{NE} \sigma_{ij} dV_k = \frac{1}{V} \sum_{k=1}^{NE} \sum_{l=1}^{8} \left( \sigma_{ij} \right) V_{l}^{\text{int}}$$

(2-3)

where $NE$ is the number of element, $V_e$ is the volume of single element. In this research, 8-node solid hexahedral elements are used to model the plane stress RVE.

### 2.2.5 Modeling of Fiber Fracture

As mentioned before, in high-strain rate applications, the fiber fracture is the most dominant failure mode. Since the fiber carries most of the load, the fiber fracture contributes most to the degradation of material strength. In this research, it is assumed that the fiber fracture occurs in the perpendicular plane to the fiber axis. When a crack exists in continuum medium, the stress concentration at the crack tip is normally the quantity of interest. However, in the case of modeling fiber fracture, the quantity of interest is not stress concentration at the crack tip, but the reduction of strength due to fiber fracture. Therefore, it is unnecessary to model crack growth within the fiber. In such a simplified case, it is possible that the crack in the fiber is modeled as enriched feature of finite elements. The extended finite element method (XFEM) uses the enriched feature and is an extension of general FEM allowing the discontinuities to exist in an element by enriching degrees of freedom with special displacement functions [65]. This method is efficient especially when crack propagation is to be investigated since it does not require remeshing as fracture of fiber progresses.

Under high strain rate impact, fiber behaves as brittle material and fiber fracture occurs completely in an extremely short time period. Figure 2-5 shows the stress-strain
curve of a common carbon fiber T300 under different strain rates [66]. We can see that the curve is composed of elastic region and sudden brittle fracture. And since the degradation of strength due to fiber fracture is the focus, the propagation of the crack is not considered. Stationary crack can be defined using an enrichment command and assigning crack domain in Abaqus. When the elements are intersected by the defined stationary crack domain, the elastic stiffness and strength of that element is regarded as zero, which can be regarded as discontinuous. Figure 2-6 shows the assignment of a stationary crack and the stress field near the crack front [64].

2.2.6 Strain Rate Effect on Material Property

As mentioned earlier, this research focuses on a high strain rate impact phenomenon. Strain rate might have a big effect on the material response. High strain rates tend to favor the elastic properties of materials. Elasticity is associated with load-bearing performance as embodied in properties such as strength and stiffness. However, low strain rates favor the viscous or energy-damping aspects of material behavior. Viscous flow is associated with energy management, often referred to as impact resistance or toughness.

For composite materials, fibers are the main load-bearing elements and reliable information of the properties of fibers under high strain rate loading is important. Because of technical difficulties in high-strain rate tests, currently, it is difficult to obtain the dynamic properties of a single fiber directly. Since a single fiber has a diameter in the range of 6 to 8 microns, it is extremely difficult to perform high-strain rate tests in the order of 1000 s\(^{-1}\) strain rate. Chi et al. [67] proposed an approach for determining the static properties of single fiber by measuring those of fiber bundles. Xia et al. [68] extended the method to dynamic state and first successfully performed tensile impact
tests on fiber bundles. Their testing strain rate was up to 1100/s. One of the most popular types is carbon fiber. Table 2-1 shows mechanical properties of two common carbon fibers, T300 and M40J, at different strain rates [66]. It can be observed that for these two kinds of carbon fibers the effect of strain rate on material property can be ignorable. However, for other kinds of fibers, the effect of strain rate might be very prominent. Figure 2-7 shows the relationship between strain rate and the ultimate strength of M40J, T300, E-glass and Kevlar49 fiber bundles [66]. It can be concluded that M40J and T300 are strain rate insensitive materials while E-glass and Kevlar49 are sensitive to strain rate.

The matrix phase for fiber reinforced composites can be a metal, polymer or ceramic. Generally, the matrix works as binding materials that supports and protects fibers. And metals and polymers are usually used as a matrix because of ductility. However, under high strain rate impact, ductile materials tend to behave as a brittle material. Figure 2-8 shows experimental tensile stress-strain curves for PR520 resin, which is commonly used as a matrix, at different strain rates [69]. Figure 2-8 indicates that as strain rate increases, ductility tends to vanish.

For both fiber and matrix, linear elastic model will be used for simplicity because both materials show brittle behavior under high-strain rate. As mentioned in previous section, fracture of fiber will be modeled using extended finite element method. Damage and fracture of matrix is not the focus here since fiber is the main load-bearing element. In fact, the failure strength of fiber is about 30 times higher than that of matrix, and the volume fraction of fiber is more than 60%. Therefore, ignoring matrix failure will not affect simulation results significantly.
2.3 Surrogate Modeling of Composites Constitutive Relation

Surrogate modeling is an approximation of a complex response using an explicit mathematical function. The complex response means the response that can be obtained via expensive numerical simulations or experiments. Depending on what kind of functions are used and how the function is fitted, different surrogate modeling methods are available, such as polynomial response surface [70], support vector machine [71], radial basis neural network [72], Krigging surrogate [73], etc. The objective of surrogate modeling is how to approximate the complex function accurately with a small number of samples. In most cases, it is assumed that obtaining sampling results is the most expensive either from experiments or simulation, but fitting the function is computationally cheap.

Surrogate modeling has three steps in general. In the first step, samples are generated within the range of input variables. Then either experiments or simulations are performed at each sample. Lastly, an explicit mathematical function is fitted using available sampling data.

2.3.1 Design of Experiments

Design of experiments (DOE) refers to the information-gathering techniques related to observations of a given phenomenon. Initially the word “experiment” referred to classical (e.g., physical, chemical) experiments. Nowadays running a computer simulation is also considered as a “computer experiment”. The experiment is controlled by a set of input variables and a set of output variables can be observed. The set of all feasible input combinations spans the input space. One execution of the experiment (with a specified value for all inputs) is called an experimental run.
Experimental runs are performed to draw conclusions about the studied phenomenon. To optimize the gain of information from a set of runs, one must execute these runs according to an appropriate DOE method. Various DOE approaches are available depending on different optimization criteria. Experimental design is important since it decides how to select the inputs at which to run the analysis in order to most efficiently reduce the statistical uncertainty of the prediction.

In the conventional polynomial response surface surrogate, various DOE methods have been developed, such as full factorial design, fractional factorial design, central composite design, etc. Also, optimization techniques can be utilized in DOE such that sampling points can be selected in some sense of optimum. For example, D-optimality method chooses sampling location by minimizing variance of coefficients, and G-optimality method chooses by minimizing prediction variance of the surrogate. Among various DOE methods, the property of space-filling is important; that is, the samples can evenly cover the design space as much as possible. Latin hypercube sampling (LHS) is one of the popular space-filling DOEs, which will be used here. However, it is noted that in high dimension, space-filling is often not satisfied because the number of samples is too small. For example, in 10-dimensional space, it will require more than 1000 sample just to cover all vertices of the input domain.

Latin hypercube sampling, due to McKay et al. [74], is a statistical method for generating random samples from a multidimensional distribution ensuring that all portion of the design space is represented. Consider an experiment controlled by n input variables. The input for one experimental run is a combination of a specified feasible value for each input variable. The input space is a n dimensional space. And
we can afford m experimental runs. We wish to sample m points in the n dimensional input space. The Latin hypercube sampling strategy can be explained as follows:

1. Divide the interval of each dimension into m non-overlapping intervals having equal probability (e.g. for uniform distribution, the intervals should have equal size).
2. Sample randomly from the distribution a point in each interval in each dimension.
3. Pair randomly (equal likely combinations) the point from each dimension.

A randomly generated Latin hypercube design may not be desired: the variables may be highly correlated or the design may not have good space-filling properties. Correlation between inputs should be reduced so that we can distinguish between the effects of the input variables. If we use a design to develop prediction model, the prediction will be poor in the unexplored areas. Thus spacing-filling property is preferred since we want to explore larger area in the input space. There are procedures to find good designs by minimizing the pairwise correlations or maximizing the minimum distance between points.

Iman and Conover [75], Owen [76], and Tang [77] proposed to find designs minimizing correlations among input variables. Morris and Mitchell [78] proposed to find the best LHS designs by maximizing the minimum distance between the points. The minimum pairwise correlation between the input variables and the maximum distance between the points are both good criteria for finding optimal LHS designs.
In this research, input variables are six components of averaged strain from macro-scale analysis. 100 samples are generated using LHS sampling. For each strain component, the range is from -0.05 to 0.05.

2.3.2 Surrogate Modeling

In this research, we want to construct surrogate models as approximations to constitutive relations. The input variables of the surrogates would be six strain components. And six surrogates are needed to predict individual stress components. To construct a surrogate, initial samples are selected using a DOE method. The number of samples selected depends on the available budget of expensive experiments and/or simulations. Experiments and/or simulations can be performed on these samples. Then with these samples as input and their corresponding experiment and/or simulation results as output, a surrogate model can be constructed as a mapping of input to output. Some of the popular surrogate models are polynomial response surface, kriging, support vector machines and radial basis neural networks.

As mentioned above, we use Latin hypercube sampling strategy to generate different combinations of strain components at which to run the simulations in Abaqus and calculate the average stresses. In Abaqus, in order to apply random strain values, equation constraint is used in python script to control translational degrees of freedom of all the nodes on the boundary.

With strain values as input and stress values as output, we can construct a surrogate for each stress component. Previously we have already mentioned that crack propagation in the fiber is not going to be investigated, only the degradation due to fiber fracture is the focus. In practice, the fiber fracture is a discontinuous phenomenon where the response of plane stress RVE abruptly changes. Therefore, it would be hard
a single surrogate can model both intact state and fractured state of fiber because the fundamental assumption is surrogate modeling is that the response is a smooth function of input variables. Instead of using a single surrogate to model the both state, we will have two plane stress RVE models with intact fiber and totally fractured fiber respectively, thus for each stress component two surrogates will be constructed.

When two surrogate models are used to determine two different states of plane stress RVE, we need a criterion to determine when given certain strain values as input which plane stress RVE model should be called, i.e. we need a criterion to determine when fiber fracture happens. First we assume that axial stress, which leads to fiber fracture, is determined by axial strain only. To verify the accuracy of this assumption, we use LHS to generate samples of inputs, run the analysis, calculate the average stress and project all points on $\varepsilon_{33}/\sigma_{33}$ plane. Here, 3 stands for the axial direction. Figure 2-9 shows the data points and linear regression. However, it is clear that the error is not ignorable. The RMS error is 100.3, 10.93% of the average value of $\sigma_{33}$. Notice that when $\varepsilon_{33}$ is zero, the value of the fitted linear function is about 250, which means that we cannot ignore the contribution of other strain components to axial stress.

This happens because when an axial deformation occurs, transverse deformation also occurs due to Poisson’s effect. Taking Poisson’s effect into consideration, instead of using $\varepsilon_{33}$ directly, we should use an equivalent $\bar{\varepsilon}_{33}$,

$$\bar{\varepsilon}_{33} = V_{13}\varepsilon_{11} + V_{23}\varepsilon_{22} + \varepsilon_{33} \quad (2-4)$$

where $V_{13}$ and $V_{23}$ are effective Poisson’s ratios obtained from homogenization of elastic behaviors. Now project all points on $\bar{\varepsilon}_{33}/\sigma_{33}$ plane. Figure 2-10 shows the modified data points and linear regression.
With $\bar{e}_{33}$, the RMS error reduces to 40.857, 4.45% of the average value of $\bar{\sigma}_{33}$. And when $\bar{e}_{33} = 0$, the value of the linear function is about 91MPa. It is accurate enough to use the equivalent axial strain as the fiber fracture criterion. By comparing $\bar{e}_{33}$ with a certain critical value, we can decide which plane stress RVE model should be called so that all the inputs can be divided into two groups and two surrogates can be constructed for each stress component.

Before implementing the surrogate models in material subroutine, the accuracy of the surrogates need to be examined. Table 2-2 shows the PRESS errors of the fitted kriging surrogates. Those surrogates were trained using 100 samples generated using LHS sampling. From Table 2-2, we can see that the fitted surrogates are very accurate.

2.3.3 Total Strain versus Incremental Strain

As mentioned before, the surrogate model takes the six components of strain as inputs and calculates six components of stress as outputs. In the viewpoint of computational mechanics, it means ‘total’ strains are used to calculate ‘total’ stresses. It sounds straightforward, but in practical application, it causes several issues. First, in nonlinear finite element analysis, stresses are incrementally updated using incremental strains. If we develop our own finite element analysis program, it is possible to make total strain information available. But, when commercial programs are used, most of cases, the users do not have access to this information.

In LSDYNA, in order to calculate the total strain, deformation gradients need to be used. To make the deformation gradient available for bricks and shells in the user-defined material subroutines, the variable IHYPER on the material card should be set to 1. The deformation gradient components F11, F21, F31, F12, F22, F32, F13, F23 and
F33 can then be found in the history variables array in positions NHV+1 to NHV+9, i.e., the positions coming right after the requested number of history variables.

One of the key issues when making the material subroutine is the choice of strain measure. The candidates are Lagrangian strain and Eulerian strain. They are calculated by following formulas

\[ E = \frac{1}{2}(F^TF - I), \quad e = \frac{1}{2}\left[I - (FF^T)^{-1}\right] \] (2-5)

where \( E \) is the Lagrangian strain, \( e \) is the Eulerian strain, \( F \) is the deformation gradient and \( I \) is the identity matrix. Since different fiber orientation is defined for each integration point, the local coordinate system option has to be invoked (IORTHO=1), then the deformation gradient is transformed to this local system prior to entering the user-defined material routine according to

\[ \bar{F} = QF \] (2-6)

where \( Q \) refers to a transformation between the current global and material frames. If we choose Lagrangian strain, then with the coordinate transformation

\[ \bar{E} = \frac{1}{2}(\bar{F}^T\bar{F} - I) = \frac{1}{2}(F^TQ^TQF - I) = \frac{1}{2}[F^T(Q^TQ)F - I] = \frac{1}{2}(F^TF - I) = E \] (2-7)

The transformation is actually cancelled out. Such problem does not exist for Eulerian strain, and that is why we choose Eulerian strain.

Other things that need to be noticed are the sequence of components of deformation gradient stored in the history variables array in positions NHV+1 to NHV+9, the different sequence of stress components in different commercial software and the difference in coordinate systems used in microscale model and macroscale model.
In addition, commercial programs require the total stress to be calculated by using total stress from the previous increment and adding incremental stress at the current increment. The stresses are not updated by simply accumulating the effect of incremental strains. Instead, the effect of rigid body rotation is included at every increment. Therefore, the output stresses from surrogate models should be modified to calculate incremental stress. To combine total strain with incremental form, the following incremental formulation is used.

\[
\text{Surrogates: } \sigma = f(\epsilon) \\
\text{At time } t: \quad \sigma' = f(\epsilon') \\
\text{At time } t+1: \quad \sigma'^+ = f(\epsilon'^+) \\
\Rightarrow \sigma'^+ = \sigma' + f(\epsilon'^+) - f(\epsilon') \quad (2-8)
\]

2.4 Results and Discussion

We compare our proposed framework with sequential multiscale modeling approach by comparing two material models, Mat22 and Umat45, in LS-DYNA. Mat22 is a built-in orthotropic material model with brittle failure for composites. With material constants defining Mat22 calculated using homogenization technique, Mat22 represents sequential approach. Umat45 is a user-defined material subroutine and within the subroutine we use surrogates to update stresses. Umat45 represents our proposed surrogate-based approach. Test results are also used to validate the approach.

2.4.1 Material Properties of Fiber and Matrix

The composite material tested has two constituents, Advantex and KER9100. The measured average fiber volume fraction is 56.73%. We use both Mat22 and Umat45 to model the material.
Advantex is a type of glass fiber. It can be modeled as linear elastic material with 81GPa as Young’s modulus and 0.22 as Poisson’s ratio.

KER9100 is a type of epoxy resin. Figure 2-11 shows the stress/strain curve of KER9100 under uniaxial tension. Matrix is modeled as linear elastic perfectly plastic material with 3084MPa as Young’s modulus, 0.398 as Poisson’s ratio and 66.9MPa as yield stress.

2.4.2 Parameters of Mat22

Material type 22 in LSDYNA is an orthotropic material with optional brittle failure for composites. It can be defined following the suggestion of Chang and Chang [79]. Three failure criteria are possible to use, i.e. matrix cracking failure criteria, compression failure criteria and fiber breakage failure criteria. The definition of those failure criteria need strength values from tests.

Other than that, the definition of material model Mat22 also requires several elastic constants, including stiffness values and Poisson’s ratios. The effective properties of unidirectional fiber reinforced composites can be obtained using plane stress RVE model and homogenization technique. The unidirectional fiber reinforced composites can be regarded as orthotropic material and the stress/strain relation can be represented as below.

$$\begin{bmatrix}
\bar{\sigma}_{xx} \\
\bar{\sigma}_{yy} \\
\bar{\sigma}_{zz} \\
\bar{\sigma}_{xy} \\
\bar{\sigma}_{yz} \\
\bar{\sigma}_{xz}
\end{bmatrix}_{\text{eff}} = \begin{bmatrix}
\bar{\varepsilon}_{xx} \\
\bar{\varepsilon}_{yy} \\
\bar{\varepsilon}_{zz} \\
\bar{\varepsilon}_{xy} \\
\bar{\varepsilon}_{yz} \\
\bar{\varepsilon}_{xz}
\end{bmatrix}_{\text{eff}}$$

(2-9)

Here, $[\bar{C}]_{\text{eff}}$ is a 6x6 stiffness matrix. By giving a specific combination of strain components, the components of the stiffness matrix can be obtained. For example,
when $\varepsilon_{xx} = 1$ and all other strains are zero, the volume-averaged stresses become the first column of the stiffness matrix. By repeating this procedure six times, i.e. controlling one of the strain component to be 1 while others are zero, we would be able to obtain the whole stiffness matrix. We can take the inverse of the stiffness matrix to get the compliance matrix. We can then calculate the effective elastic properties from the compliance matrix.

\[
[S] = [\tilde{C}]_{\text{eff}}^{-1} = \begin{bmatrix}
1 & -\nu_{21} & -\nu_{31} & 0 & 0 & 0 \\
\frac{E_{11}}{v_{12}} & \frac{E_{22}}{1} & -\nu_{32} & 0 & 0 & 0 \\
\frac{E_{11}}{v_{13}} & \frac{E_{22}}{v_{23}} & \frac{E_{33}}{1} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{G_{12}}{1} & 0 \\
0 & 0 & 0 & 0 & \frac{G_{13}}{1} \\
0 & 0 & 0 & 0 & 0 & \frac{G_{23}}{1}
\end{bmatrix}
\] (2-10)

Using this method, the obtained values are shown in Table 2-3.

2.4.3 Strain Rate Effect

As mentioned before, glass fiber is sensitive to strain rate. The response of epoxy resin also changes with strain rate. However, since fiber carries most of the load, it is safe to ignore the effect of strain rate on matrix. We will use the form of Johnson-Cook model [80] to include the strain rate effect in the material subroutine. The Johnson-Cook model is purely empirical and gives the following relation for the yield stress:

\[
\frac{\sigma_y}{\sigma_{y0}} = 1 + C \cdot \ln \left( \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_{p0}} \right)
\] (2-11)

Here, $\sigma_y$ is the yield stress, $\dot{\varepsilon}_p$ is the plastic strain rate, $\sigma_{y0}$ and $\dot{\varepsilon}_{p0}$ are the reference value.
We can use the form of Johnson-Cook model to consider the strain rate effect on material properties of Advantex. Since Advantex has similar mechanical property with E-glass, we can estimate the strain rate effect on Advantex by using the data of E-glass response under different strain rate. Table 2-4 shows how strain rate affects material properties of E-glass [81].

Take the strength of E-glass under different strain rate for instance. Use strain rate of 90s\(^{-1}\) as the reference value. The constant C can be found by minimizing discrepancy from experimental data. Figure 2-12 shows the comparison between the experimental data and the surrogate. And we can get Equation 2-12.

\[
\frac{\sigma}{\sigma_{r0}} = 1 + 0.1323 \ln\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)
\]  

(2-12)

2.4.4 Comparison of Behavior of Material Models

Ten composites specimens were prepared and uniaxial tension tests were performed. Five specimens were tested in longitudinal direction while the other five were tested in transverse direction. And the test results are shown in Figure 2-13 and 2-14. Based on the test results, linear response surface is chosen as the surrogate since linear response surface can serve as a good approximation to the test data and it is easy to implement. So the stress can be calculated using the Equation 2-13.

\[
\{\sigma\} = [D]\{\varepsilon\} + \{C\}
\]  

(2-13)

Here, [D] is the coefficient matrix and is a constant vector.

For the analysis of composite laminates, classical laminate theory is a popular approach. This approach treats composite laminates as a type of plate or thin-shell structure and calculate their stiffness properties by integration of in-plane stress through the thickness. The ply materials obey Hooke’s law and hence stresses and strains can
be related by a system of linear equations. This is the major similarity with our approach. The difference is our approach calculates the stresses in each ply so that we can deal with the failure of each ply independently and the same failure criterion can be used regardless of the lay-up configuration of the laminates. Another advantage is our approach is not limited to the analysis of thin plate since all six stress components are updated using surrogates.

Figure 2-15 and 2-16 show the comparison of material response of two approaches in longitudinal and transverse directions, respectively. In longitudinal direction, both approaches show good agreement with experimental results. After fiber fractures, Mat22 loses load-carrying capacity completely and the stress value drops to zero, while Umat45 can still carry some load since matrix has higher failure strain compared to fiber. In transverse direction, because of fiber-matrix interfacial debonding and matrix cracking, failure occurs very early. Umat45 is able to capture this drop in stress value while the response of Mat22 continues to increase after failure occurs.

Figure 2-17 shows the comparison of Mat22 and Umat45 behaviors with [0˚ 90˚] layup configuration. For the stress/strain curve of Umat45, the change in slope indicates the failure of 90˚ ply and the maximum stress is half of the strength in longitudinal direction. Compared with Mat22, Umat45 can better capture the major failure mechanisms occurred at the micro-scale.

Figure 2-18 shows that Umat45 also has the ability to take strain rate effect into consideration. Strain rate affects material behavior through affecting fiber stiffness and strength. With the increase of strain rate, both the slope and failure strain of stress/strain curve of Umat45 increase, resulting in a higher strength.
Besides the modeling of composite materials, another challenge in designing composite structures is the large level of uncertainty in the mechanical properties of composites. Here, we used our microscale model and aforementioned homogenization technique to investigate the effect of volume fraction on the effective mechanical properties of composites by varying the value of volume fraction. Figure 2-19 shows the results. From Figure 2-19, we can observe that the volume fraction has a significant effect on all the elastic constants. The variation in volume fraction would cause the uncertainty in mechanical properties. It would be dangerous to ignore the variation and assume a constant volume fraction in the design process. This leads to another important topic, uncertainty quantification in Chapter 3.
### Table 2-1. Mechanical properties of T300 and M40J at different strain rates.

|      | $\dot{\varepsilon}$ (s$^{-1}$) | E (GPa) | $|\Delta E/E|$ | $\varepsilon_b$ (100%) | $|\Delta \varepsilon_b/\varepsilon_b|$ | $\sigma_b$ (GPa) | $|\Delta \sigma_b/\sigma_b|$ |
|------|---------------------------------|---------|----------------|--------------------------|-----------------------------------|-----------------|--------------------------|
| M40J | 0.001                           | 357.9   | 2.3%          | 1.26                     | 4.1%                              | 3.339          | 3.2%                     |
|      | 100                             | 359.6   | 2.5%          | 1.28                     | 2.2%                              | 3.336          | 2.6%                     |
|      | 500                             | 360.1   | 2.0%          | 1.29                     | 2.3%                              | 3.354          | 1.2%                     |
|      | 1300                            | 359.1   | 2.1%          | 1.29                     | 3.4%                              | 3.347          | 2.6%                     |
|      | Average value                   | 359.2   | ---           | 1.28                     | ---                               | 3.344          | ---                      |
| T300 | 0.001                           | 223.2   | 4.5%          | 1.35                     | 4.1%                              | 2.387          | 3.6%                     |
|      | 100                             | 227.4   | 3.7%          | 1.32                     | 4.0%                              | 2.415          | 3.2%                     |
|      | 500                             | 223.5   | 3.4%          | 1.34                     | 3.6%                              | 2.404          | 2.8%                     |
|      | 1300                            | 225.6   | 4.1%          | 1.34                     | 3.7%                              | 2.418          | 3.4%                     |
|      | Average value                   | 224.9   | ---           | 1.34                     | ---                               | 2.406          | ---                      |

### Table 2-2. PRESS errors of surrogates of each stress component

<table>
<thead>
<tr>
<th>$\sigma_{11}$</th>
<th>$\sigma_{22}$</th>
<th>$\sigma_{33}$</th>
<th>$\sigma_{12}$</th>
<th>$\sigma_{13}$</th>
<th>$\sigma_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean value/MPa</td>
<td>443</td>
<td>443</td>
<td>918</td>
<td>216</td>
<td>200</td>
</tr>
<tr>
<td>PRESS error</td>
<td>5.31e-4</td>
<td>3.28e-4</td>
<td>9.46e-4</td>
<td>1.34e-4</td>
<td>1.75e-4</td>
</tr>
</tbody>
</table>

### Table 2-3. Homogenized elastic constants

<table>
<thead>
<tr>
<th>$E_{11}$/MPa</th>
<th>$E_{22}$/MPa</th>
<th>$E_{33}$/MPa</th>
<th>$N_{21}$</th>
<th>$N_{31}$</th>
<th>$N_{32}$</th>
<th>$G_{12}$/MPa</th>
<th>$G_{23}$/MPa</th>
<th>$G_{31}$/MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>46197.95</td>
<td>12720.22</td>
<td>14162.64</td>
<td>0.0953</td>
<td>0.082</td>
<td>0.3838</td>
<td>2231</td>
<td>3668.62</td>
<td>3589.29</td>
</tr>
</tbody>
</table>

### Table 2-4. Mechanical properties of E-glass bundles at different strain rate

<table>
<thead>
<tr>
<th>Strain rate</th>
<th>$\dot{\varepsilon}$ (s$^{-1}$)</th>
<th>90</th>
<th>300</th>
<th>800</th>
<th>1100</th>
<th>1300</th>
<th>1700</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strength</td>
<td>$\sigma_b$ (GPa)</td>
<td>2.15</td>
<td>2.50</td>
<td>2.75</td>
<td>2.85</td>
<td>2.93</td>
<td>2.99</td>
</tr>
<tr>
<td>Failure strain</td>
<td>$\varepsilon_b$ (%)</td>
<td>3.70</td>
<td>4.00</td>
<td>4.30</td>
<td>4.40</td>
<td>4.41</td>
<td>4.11</td>
</tr>
<tr>
<td>Stiffness</td>
<td>$E$ (GPa)</td>
<td>69.397</td>
<td>74.832</td>
<td>76.736</td>
<td>77.30</td>
<td>78.00</td>
<td>84.40</td>
</tr>
</tbody>
</table>
Figure 2-1. Illustration of multi-scale modeling

Figure 2-2. RVE of unidirectional fiber-reinforced composites
Figure 2-3. Heterogeneous structure composed of plane stress RVE piled up. A) Y direction. B) Z direction

Figure 2-4. Heterogeneous structure model with plane stress RVE
Figure 2-5. Stress-strain curve of T300 under different strain rates

Figure 2-6. Transverse direction crack in fiber
Figure 2-7. Effect of strain rate on ultimate strength of fiber bundles

Figure 2-8. Experimental tensile stress-strain curves for PR520 resin at strain rates of 5x10^-5/s (low rate), 1.4/s (medium rate) and 510/s (high rate)
Figure 2-9. $\varepsilon_{33}/\sigma_{33}$ data points and linear regression

Figure 2-10. $\bar{\varepsilon}_{33}/\sigma_{33}$ data points and linear regression
Figure 2-11. Stress/strain curve of KER9100 under uniaxial tension

Figure 2-12. Fit to strength of E-glass under different strain rates using log function
Figure 2-13. Tensile test in longitudinal direction

Figure 2-14. Tensile test in transverse direction
Figure 2-15. Comparison of Mat22 and Umat45 response in longitudinal direction with experimental data

Figure 2-16. Comparison of Mat22 and Umat45 response in transverse direction with experimental data
Figure 2-17. Comparison of Mat22 and Umat45 response with [0° 90°] layup configuration

Figure 2-18. Comparison of Mat22 and Umat45 response in longitudinal direction under different strain rate
Figure 2-19. Effect of volume fraction on the effective mechanical properties of composites.
CHAPTER 3
UNCERTAINTY QUANTIFICATION AND REDUCTION IN MULTISCALE MODELING
OF COMPOSITES USING BAYESIAN INFERENCE

Uncertainty analysis of unidirectional fiber reinforced composites is very
challenging due to various sources of uncertainty, such as uncertainties in fiber and
matrix properties, fiber/matrix interfacial property, voids and porosity and fiber
misalignment. And the textile structure makes the uncertainty analysis of plain weave
fabric even more complex. Due to the high level of uncertainty, too many tests are
required to estimate uncertainty in structural elements which are very costly.

In traditional metallic structures, such as aluminum, the material properties
including statistical variability (aleatory uncertainty) are estimated using coupon tests,
where 50 ~ 100 coupons are used to estimate A- or B-basis allowables of material
strength. Since the material properties are maintained for the upper level of the building-
block, the same allowables can be used for structural elements or components.
Therefore, element and component tests focus on detecting design errors (epistemic
uncertainty), rather than material variability. That is why only a handful number of tests
are performed in element and component level.

On the other hand, for composite materials, it is difficult to separate aleatory
uncertainty from epistemic uncertainty. In particular, the variability (aleatory uncertainty)
in material properties in a lower scale is different from the variability in the upper scale.
For example, in the fiber level, the variability is mostly due to the distribution of failure
strength of the fiber. In the prepreg level, additional variability is added due to variable
volume fraction as well as variability in the curing process. In the composite panel level,
additional variability is included due to stacking process. Therefore, it is the current
practice that material variability and design errors are tested at the same time in the
element and component level, which requires many specimens. Considering structural element and component tests are much more expensive than coupon tests, the time and cost can significantly increase.

An important contribution of the proposed research is to reduce the required number of tests in structural element and component level. The objective is to establish a framework of estimating uncertainty in composite panel using a similar number of tests as in aluminum materials; i.e., about 50 ~ 100 tests in fiber and matrix level, 4 ~ 5 tests in prepreg and composite panel level.

We propose to propagate uncertainty starting from a lower scale to the upper scale, in our case fiber and matrix level to structural components. Tests and simulation results at different scales can be used to effectively reduce epistemic uncertainty via Bayesian inference. In this approach, with uncertainty propagated from lower scale served as prior, the number of tests required can be reduced.

The key idea in uncertainty propagation and reduction in multi-scale environment is surrogate modeling and Bayesian inference. When a numerical method, such as finite element analysis, is used to upscaling the scale, surrogate modeling is employed to approximate the upscaling process with a reasonable number of simulations. Using the surrogate model, uncertainty in the lower scale can be propagated to the upper scale be generating many samples. In the upper scale, the uncertainty obtained using the surrogate model is used as a prior distribution. The uncertainty in the upper scale is further reduced by additional tests using Bayesian inference.
In this research, we will focus on the strength prediction of plain weave fabric in high strain rate application. But, the basic concept can be applicable to other types of fabric.

Woven fabric composites are used in composites structures as an alternative to traditional unidirectional fiber reinforcing laminates, with applications in various fields such as automotive and aerospace engineering. The interest in this type of composites has increased due to both the advances made in textile industry (the use of high performance fibers in high quality weaves), and the advantages conferred by the woven reinforcements compared to fiber lay-up (easier manipulation and lay-up during composite material manufacturing, good drapability properties that allows the use of woven reinforcements in complex mold shapes, increased impact resistance and damage tolerance of the composite material.) [82]

Woven fabrics are produced by the interlacing of warp (0°) yarns and weft (90°) yarns in a regular pattern or weave style. The fabric's integrity is maintained by the mechanical interlocking of the yarns. Drape (the ability of a fabric to conform to a complex surface), surface smoothness and stability of a fabric are controlled primarily by the weave style. For plain weave fabric, each warp yarn passes alternately under and over each weft yarn. The fabric is symmetrical, with good stability and reasonable porosity. However, it is the most difficult of the weaves to drape, and the high level of yarn crimp imparts relatively low mechanical properties compared with the other weave styles.

3.1 The Bayesian Approach to Probability and Statistics

The Bayesian probability of an event x is a person’s degree of belief in that event. Whereas a classical probability is a physical property of the world (e.g., the
probability that a coin will land heads), a Bayesian probability is a property of the person who assigns the probability (e.g., your degree of belief that the coin will land heads) [83]. And Bayesian inference is a method of updating the degree of belief as more evidence or information becomes available. Bayesian inference derives the posterior probability as a consequence of a prior probability and a likelihood function derived from a statistical model for the observed data.

To illustrate the Bayesian approach, consider a coin tossing problem. Suppose we flip the coin N+1 times. From the first N observations, we want to determine the probability of heads on the N+1th toss. To examine the Bayesian analysis of this problem, we need some notation. We denote a variable by an upper-case letter (e.g., X, Y), and the state of a corresponding variable by that same letter in lower case (e.g., x, y). We define Θ to be a variable whose values θ correspond to the possible true values of the physical probability. θ is often referred to as a parameter. In this problem, θ is the probability of getting heads. We express the uncertainty about Θ using the probability density function \( p(\theta | \xi) \). This denotes the probability density that \( \Theta = \theta \) of a person with prior information \( \xi \). We use \( D = \{X_1 = x_1, ..., X_N = x_N\} \) to denote the set of our observations.

Bayes’ theorem can be expressed in terms of the continuous probability distribution with probability density function (PDF), which is more appropriate for the purpose of updating a distribution. Let \( p(\theta | \xi) \) be a PDF of parameter \( \theta \) with a given prior knowledge of \( \xi \). If the test measures a value \( D \), it is also a random variable, whose PDF is denoted by \( p(D | \xi) \). Then, the joint PDF of \( \theta \) and \( D \) can be written in terms of \( p(\theta | \xi) \) and \( p(D | \xi) \), as
\[ p(D, \theta|\xi) = p(D|\xi) p(\theta|D, \xi) = p(\theta|\xi) p(D|\theta, \xi) \] (3-1)

For example, \( \theta \) can be a failure strength of a coupon, which has epistemic uncertainty, and \( D \) is a test result of failure strength. Normally test results have measurement variability, and thus, \( D \) is considered as a random variable.

Using the above identity, the original Bayes’ theorem can be extended to the posterior probability distribution of \( \Theta \) given \( D \) and prior knowledge \( \xi \)

\[ p(\theta|D, \xi) = \frac{p(\theta|\xi)p(D|\theta, \xi)}{p(D|\xi)} \] (3-2)

where

\[ p(D|\xi) = \int p(D|\theta, \xi)p(\theta|\xi)d\theta \] (3-3)

is the marginal distribution test distribution. Considering that the area under the PDF is one, the denominator may not play important role. Therefore, for a given prior distribution \( p(\theta|\xi) \), the only important information is the likelihood, \( p(D|\theta, \xi) \). The likelihood function is the probability density value of test \( D \) given \( \theta \).

In the case of coin toss, the likelihood function, \( p(D|\theta, \xi) \), takes the binomial distribution. Therefore, the posterior distribution can be expressed as

\[ p(\theta|D, \xi) = \frac{p(\theta|\xi)\theta^h(1-\theta)^t}{p(D|\xi)} \] (3-4)

where \( h \) and \( t \) are the number of heads and tails observed in \( D \). The probability distributions \( p(\theta|\xi) \) and \( p(\theta|D, \xi) \) are commonly referred to as the prior and posterior.

Finally, with the posterior distribution of \( \Theta \), we can calculate the probability of heads for \( N+1 \)th toss.

\[ p(X_{N+1} = \text{heads} | D, \xi) = \int \theta p(\theta|D, \xi) d\theta \equiv E_{p(\theta|D, \xi)}(\theta) \] (3-5)

here, \( E_{p(\theta|D, \xi)}(\theta) \) denotes the expectation of \( \Theta \) with a distribution of \( p(\theta|D, \xi) \).
3.2 Proposed Framework

Figure 3-1 shows the proposed multiscale framework of modeling plain weave fabric. Three scales are considered, i.e. fiber, yarn & prepreg and composite plate. In the fiber scale, the behavior of individual fiber is modeled and tested. The yarn is a bundle of about 3,000 fibers together, while prepreg is a fabric woven by yarns. The composite plate is composed of a stack of several prepreg.

It is possible that yarn and prepreg can be separated, but we decided to combine them together because tests in yarn bundle is difficult due to designing a special grip to hold 3,000 fibers individually with equal forces. In the fiber scale, single fiber tension tests are performed multiple times to obtain the statistical knowledge of fiber properties. In yarn & prepreg scale, both simulation and tests are performed. Tests and simulation results can be used to effectively reduce uncertainty via Bayesian approach. With simulation results serving as prior and test results serving as likelihood, a posterior can be generated using Bayesian method. The generated posterior can be used as input for the simulation in the next scale. At the composite plate scale, with finite element analysis and Monte Carlo simulation, the distribution of plate strength can be predicted. The predicted distribution can then be used to validate the framework by comparing with test data.

3.2.1 Fiber Scale

In the fiber scale, single fiber filament tension test is used to measure the mechanical properties of fiber, i.e. stiffness and strength. Test is repeated 29 times to provide information on the variability of the material properties. This information can be used as input to the next scale.
The fiber tested is T300 carbon fiber. Single fiber filament tension tests are performed following ASTM C1557-14 [84]. To prepare a specimen, a fiber is extracted randomly from a bundle or from a spool. The fiber is first fixed on a paper mounting tab using glue tape and then further fixed using adhesive. The shape of the specimen is shown in Figure 3-2. After the adhesive is fully cured, the tab can be mounted in the test machine. Before applying a load, both sides of the tab need to be cut or burned very carefully at mid-gage, as shown in Figure 3-3. The fiber is then stressed to failure at a constant displacement rate. The testing machine is shown in Figure 3-4. A valid test result is considered to be the one in which fiber failure doesn’t occur in the gripping region but around the mid-gage.

Diameters of the fibers need to be given to calculate strain and stress. In order to obtain a more accurate estimation of the uncertainty of the mechanical properties of fibers, the diameter of each fiber is measured using microscope. Figure 3-5 shows the histogram of fiber diameters. It is appropriate to describe the variability of fiber diameters using normal distribution. And the mean of the measurements is 7.13µm, which agrees well with the data provided by the manufacturer 7µm.

After measuring the diameter of each fiber, 29 specimens are tested and stressed to failure. Figure 3-6 and Table 3-1 show the test results. All fibers show a linear elastic behavior, followed by a brittle failure. We noticed that for all of the curves, the initial stresses are not zero. This is because before automatically loading the fibers to failure, we need to manually load the fibers so that the fibers are under pretension. Despite a small variation in elastic stiffness, there is large uncertainty in tensile strength and strain at tensile strength. This could be due to possible surface damage of fibers or
the axial misalignment of the fiber along the line of action of the machine. Since the fiber is extremely thin, it is impossible to recover the failed fiber after test. This high level of uncertainty will propagate to the next scale, i.e. yarns. However, since a yarn is composed of several thousand fiber filaments, the behavior of yarn tends to be the average behavior of all the fibers. So the uncertainty of yarn stiffness properties would be reduced a lot if the contributions of other factors to the variability are not considered. This is an important aspect in multi-scale uncertainty propagation, where the high level of uncertainty is averaged in the upper scale, and thus, the uncertainty is significantly reduce.

For the case of elastic stiffness, the above mentioned averaging uncertainty can easily be understood. However, in the case of failure strength, it is a more difficult to explain using the concept of averaging because the failure is dominated by the weakest member. However, the failure of a weak failure does not mean the failure of entire fiber bundle. Therefore, more detailed study is required, which will be discussed in the next section.

The histograms of fiber strength and stiffness are shown in Figure 3-7. The distribution of fiber strength can be estimated from the test data. However, since the true distribution parameters are estimated with a finite number of tests, the estimated parameters have sampling uncertainty. Thus, it is natural to consider these parameters as distributions rather than deterministic values. The estimated fiber strength essentially becomes a distribution of distributions [50]. The distribution of fiber strength can be obtained using a double-loop Monte Carlo simulation. We assume that the fiber strength follows a normal distribution with a true mean \( \mu \) and a true standard deviation \( \sigma \). The
sample mean and sample standard deviation calculated from a finite number of tests are \( \bar{Y} \) and \( s \). The true mean and true standard deviation can be sampled from t distribution and chi-squared distribution using Equation 3-6. Here, \( n \) is the number of data.

\[
\frac{\bar{Y} - \mu}{s / \sqrt{n}} \sim t(n-1)
\]

\[
\frac{(n-1)s^2}{\sigma^2} \sim \chi^2(n-1)
\]

Then fiber strength can be sampled from samples of true mean and true standard deviation. The estimated distributions with and without sampling uncertainty are shown in Figure 3-8. From the comparison we can observe that by considering sampling uncertainty the estimated distribution has a larger variability. Since 29 samples are available for the fiber, the sampling uncertainty is relatively small compared to variability of failure strength itself. Since the fiber tension test is cheapest test in the building-block process, it would make sense to perform enough tests to reduce the sampling uncertainty.

### 3.2.2 Yarn/prepreg Scale

In yarn scale, several thousand fiber filaments are bundled together. Yarns can be regarded as unidirectional fiber reinforced composites and analytical equations can be used to assess the elastic properties of yarns. The only difference is that it is necessary to consider the volume fraction of fibers in a yarn, because the circular cross-section of fiber cannot fill the entire space in the yarn. Equation 3-7 are taken from Chamis [85] to estimate the elastic properties of yarns. In Equation 3-7, the fiber volume fraction is \( V_f \), and matrix volume fraction is \( V_m \). In practical manufacturing process, it is
possible that there is some void within the yarn, but it is assumed that the empty space between fibers are filled by matrix completely, such that $V_f + V_m = 1$.

$$E_i = V_f E_{f,i} + V_m E_m$$
$$\nu_{12} = \nu_{13} = V_f \nu_{f/12} + V_m \nu_m$$
$$E_2 = E_3 = \frac{E_m}{1 - \sqrt{V_f} \left(1 - \frac{E_m}{E_f} / E_{f,2}\right)}$$
$$G_{12} = G_{13} = \frac{G_m}{1 - \sqrt{V_f} \left(1 - \frac{G_m}{G_{f,12}} / G_{f,12}\right)}$$
$$G_{23} = \frac{G_m}{1 - \sqrt{V_f} \left(1 - \frac{G_m}{G_{f,23}} / G_{f,23}\right)}$$
$$\nu_{23} = \frac{E_2}{2G_{23}} - 1$$

Here, $E_m$ and $\nu_m$ are the stiffness and Poisson’s ratio of matrix. $E_f$, $G_f$ and $\nu_f$ are the stiffness, shear modulus and Poisson’s ratio of fiber. 1, 2 and 3 represent longitudinal transverse and through-the-thickness direction, respectively. In microscale, we observed a small variation in fiber stiffness from tests. Without considering other sources of uncertainty, the variation in yarn stiffness is further reduced since yarns tend to show the average behavior of several thousand fibers. And our interest is strength rather than stiffness. So in this research, we do not consider the uncertainty in yarn stiffness.

For the yarn strength in the longitudinal direction, a statistical approach is developed to predict the maximum load-carrying capacity of yarns. This approach is implemented in Abaqus as a material subroutine VUMAT to represent the behavior of yarns. However, the statistical modeling of yarn strength is quite different from that of the yarn stiffness. For the failure strength, the averaged failure strength cannot be used because the yarn failure is controlled by the weakest fiber strength. When the yarn is
under a tensile load, the stress in individual fibers gradually increase. When the level of stress reaches to the failure strength of the weakest fiber, the weakest fiber fails first. However, the failure of the weakest fiber does not mean the total failure of the yarn. Most other fibers still can carry the load. When a fiber fails, the stiffness of the yarn is reduced because the failed fiber cannot contribute to the stiffness. Since the stiffness is reduced, the slope of the load-displacement curve will gradually be decreased. At the same time, the load carried by the failed fiber is re-distributed to all other intact fibers. The load can continuously increase until the next weak fiber is failed, where its load is re-distributed to other intact fibers. This process can continue until the yarn cannot hold a further load, which is the maximum load the yarn can support. The displacement beyond this point can cause abrupt failure of the yarn and the stress in the yarn will decrease rapidly. Even if some fractions of fibers are failed at the maximum load, the stress in the yarn is still calculated based on the total cross-sectional areas of all fibers because there is no way to count how many fibers are failed. The statistical modeling of yarn strength is quite complicated, which will be explained in this section.

Since for composite materials most of the load is carried by fiber, the only failure mechanism considered is fiber breakage. We assume that after fiber breaks in the longitudinal direction, its load-carrying capacity is lost. In other words, a fiber filament becomes void in the longitudinal direction after it breaks while in transverse and through-the-thickness direction the fiber is still intact.

The statistical nature of material properties leads to the variation in yarn strength. As load increases, some fiber filaments break, fiber volume fraction decreases while void volume fraction increases and matrix volume fraction remains the same. And the
longitudinal stiffness is reduced. Figure 3-9 shows how the fiber volume fraction is updated. With the current longitudinal strain value and the distribution of failure strain of fiber, we can calculate the percentage of fractured fibers $\alpha$. Then with the initial fiber volume fraction as $V_{f0}$, we can update the current fiber volume fraction as $(1-\alpha\%)V_{f0}$. Using the updated fiber volume fraction, we can calculate the degraded longitudinal modulus while the transverse modulus does not change. At last, stresses are updated using total strain and updated elastic constants.

We assume that fiber strength follows a normal distribution based on the fiber strength test data in the previous section. Fiber volume fraction is updated using the standard normal cumulative distribution function. Since this calculation will be done many times during computation, it is important to calculate the CDF efficiently. In addition, this will be implemented in the user material subroutine, it needs to be implemented in FORTRAN programming language. However, since there is no intrinsic function in FORTRAN to calculate the value of standard normal CDF, an approximation has to be used. For a random variable $X$ following standard normal distribution and $a>0$, the probability that $0<X<a$ is

$$P(a) = \frac{1}{\sqrt{2\pi}} \int_{0}^{a} e^{-x^2/2} \, dx$$

(3-8)

According to R. J. Bagby 1995 [86], the approximation to $P(a)$ is

$$Q(a) = \frac{1}{2} \left[ 1 - \frac{1}{30} \left[ 7e^{-a^2/2} + 16e^{-a^2(2-\sqrt{2})} + (7 + \frac{\pi}{4}a^2)e^{-a^2} \right] \right]^{1/2}$$

(3-9)

The error of this approximation in the range of $[-3, 3]$ is shown in Figure 3-10. From the values of error, we can see that this approximation is very accurate.

The developed material subroutine is tested using a uniaxial tension in longitudinal direction. The material properties of T300 carbon fiber and polyetherimide (PEI) are used, as shown in Table 3-2. The behavior is compared with the case in which
failure is not considered. The comparison is shown in Figure 3-11. From Figure 3-11, we can see that in the beginning, since there is no damage or failure, the two material models behave the same. As load increases, the two lines start to diverge because the proposed model includes the stiffness decrease due to failed fibers. The deviation continues until at a certain point the response of material model with damage drops and continue to decrease.

There are four factors influencing the material behavior. Those are fiber stiffness, mean of fiber strength, coefficient of variation of fiber strength and fiber volume fraction within the yarn. Among the four factors, fiber stiffness only affects the slope of the curve while fiber volume fraction within the yarn simply serves as a scaling factor. The effects of mean of fiber strength and coefficient of variation of fiber strength on yarn strength (maximum stress on the curve) are shown in Figure 3-12 and 3-13. As shown in Figure 3-12 and 3-13, with an increasing mean of fiber strength, yarn strength increases while the stress/strain curves are very similar. And as the coefficient of variation of fiber strength increases, yarn strength decreases while the stress/strain curve tends to have a longer tail.

In the view point of statistical characterization of yarn stiffness and strength, the uncertainty in yarn stiffness is ignored due to small uncertainty in fiber stiffness and the averaging process of more than 3,000 fibers to compose of the yarn. On the other hand, the uncertainty in fiber strength (the mean and the coefficient of variation) is used to model the nonlinear behavior of yarn strength.

In the prepreg scale, yarns are woven together to have a 2D structure. Besides mechanical properties of fiber and matrix, the crimp in yarn also affects prepreg
stiffness and strength. Therefore, it is necessary to predict the effect of woven yarns using numerical simulation. In this research, a finite element numerical model of prepreg is created based on nominal geometric dimensions and geometric variation is not considered.

The plain weave fabric in this research is Carbon prepreg CF3327. Table 3-3 shows the data provided by the manufacturer. The yarn type of both fill and warp is carbon 3K. 3K is the tow size, which means there are 3000 fiber filaments in a bundle. The average diameter of carbon fiber from measurements is 7.13µm. We can approximate the cross section of yarn as lenticular. We use half fabric thickness, which is 135µm, as the thickness of yarn. The density of warp and fill yarn is 13 count/inch. So the distance between the central lines of adjacent yarns is $25.4 \times \frac{3}{13} = 1953.85 \mu m$.

Then, we need to come up with the area of the lenticular so that we can calculate the width of the cross section.

$$\frac{\pi \left( \frac{7.13}{2} \right)^2}{V_f} \cdot 3000 = \frac{2ab}{3}$$

(3-10)

Here, $a$ is the width and $b$ is the thickness of the cross section. $V_f$ is the microscale fiber volume fraction, that is the fiber volume fraction within the yarns. However, it is very difficult to measure $V_f$ directly. We need to use Equation 3-11.

$$V_o = V_f \cdot V_g$$

(3-11)

Here, $V_o$ is the overall fiber volume fraction. $V_g$ is the mesoscale volume fraction, which is the ratio of yarn volume to fabric volume, and can be calculated from FEM model.
We need to calculate $V_o$ using the data provided by the manufacturer. The type of carbon fiber used in the fabric is T300, with a density of 1.76 g/cm$^3$. And the fabric areal weight is 208.5g/m2, with a thickness of 0.27mm. We can use Equation 3-13 to calculate the overall fiber volume fraction.

\[
\text{density of fabric: } \frac{208.5\, \text{g}}{0.027 \times 10^{-3} \, \text{cm}^3} = 0.772 \, \text{g / cm}^3
\]
\[
0.772 = 1.76 \times V_o \Rightarrow V_o = 43.86\%
\]

An iterative procedure is used to calculate the values. First, we assume a value of $V_i$. Based on the assumed $V_i$, we can use Equation 3-10 to determine the geometry of the RVE. Then we can create a FEA model, calculate the volume of the yarns and use Equation 3-12 to obtain $V_g$. At last, we use Equation 3-11 to calculate $V_i$. Compare the assumed $V_i$ and calculated $V_i$. Repeat the process until those two values are very close.

Using the iterative process, we can obtain the value of $V_i$ as 69.5%. So we would treat the yarns as unidirectional fiber reinforced composites with a fiber volume fraction of 69.5%. A FEA model of prepreg is created in Abaqus based on the calculation, as shown in Figure 3-14. This model is created using TexGen software.

With the developed material subroutine of yarns and the FEA model of prepreg, we can perform uniaxial tension test to find the strength of prepreg. The strength is defined as the maximum stress obtained as the displacement increases. As yarn strength, the prepreg strength is also affected by mean of fiber strength and coefficient of variation of fiber strength as well as fiber volume fraction.
With mean of fiber strength and coefficient of variation of fiber strength as well as yarn fiber volume fraction as input, we generate 100 samples using Latin hypercube sampling and build a kriging surrogate to predict prepreg strength \( y = f(\mu_s, CV_s, V_f) \). The effects of mean of fiber strength and coefficient of variation of fiber strength on prepreg strength predicted by built surrogate are shown in Figure 3-15 and 3-16. As the central tendency of fiber strength increases, prepreg strength also increases. And when the strength values of fibers tend to show larger variation, prepreg strength decreases.

For the purpose of uncertainty quantification, the mean strength of fiber is sampled from a normal distribution while coefficient of variation of fiber strength and yarn fiber volume fraction are sampled from uniform distributions. Using the surrogate of prepreg strength and Monte Carlo simulation, the distribution of prepreg strength can be predicted and used as prior, denoted as \( p(y) \). 18 plain weave composites specimens are prepared and tested, denoted as \( D\{y_1, y_2, ..., y_{18}\} \). Then with tests results serving as likelihood, we use Bayes’ rule to calculate the posterior probability distribution and update our knowledge of the variability of prepreg strength.

\[
p(y|D) \propto p(y) p(D|y)
\]  

(3-14)

### 3.2.3 Composite Plate Scale

In macroscale, composite plates with holes are both tested and simulated. The shape of tested specimen is shown in Figure 3-17. The diameter of the holes is 3mm. Gauge length is 50mm. And the test results are shown in Table 3-4. The distribution of plate strength can be estimated from the test data. Sampling uncertainty is included.
The composite plate with holes is also simulated using the finite element model shown in Figure 3-18. With prepreg strength as input, a linear regression surrogate model is built to predict plate strength. Then with samples from the posterior distribution of prepreg strength obtained using Bayesian approach in mesoscale, using Monte Carlo simulation, distribution of plate strength can be predicted.

3.3 Results and Discussion

In mesoscale, predicted histogram of prepreg strength using Monte Carlo simulation is shown in Figure 3-19, together with 18 test data and estimated distribution from data with sampling uncertainty. The histogram and estimated distribution from data have different mean and the estimated distribution shows less variability. Figure 3-20 shows the calculated posterior distribution of prepreg strength by combining simulation and tests using Bayes’ rule. And the means and standard deviations of prior distribution, test data and posterior distribution are shown in Table 3-5. Predicted distribution from simulation suffers from epistemic uncertainty because of numerical error and the assumptions that we made. Estimated distribution from data suffers from sampling uncertainty since we can only afford a finite number of tests. And the data itself can be lousy due to the measurement error. By combing simulation and tests using Bayesian approach, both uncertainties can be reduced and the predictive distribution of prepreg strength has smaller uncertainty.

As scale goes up, cost of tests increases dramatically. We can afford 29 tests in microscale, however, 18 tests in mesoscale would usually be expensive and time-consuming. Now suppose we only have one group of data (4 data). Figure 3-21 shows the calculated posterior using 4 data. And the means and standard deviations of the prior, data and posterior are shown in Table 3-6. Again, Bayes’ rule helps achieve a
more accurate uncertainty estimation. Figure 3-22 shows the comparison of the two cases. Compared with the estimated distribution using 18 data with prior, the estimated distribution using 4 data with prior shows different central tendency and larger uncertainty. However, compared with the estimated distribution using 18 data only, the estimated distribution using 4 data with prior shows less variation which indicates that by propagating uncertainty from lower scale and combining the propagated uncertainty with limited number of tests in the upper scale we can actually achieve more accurate uncertainty estimation than performing much more tests.

In macroscale, the distribution of plate strength is predicted using surrogate model and Monte Carlo simulation. The distribution is also estimated from test data. Figure 3-23 shows the comparison of the two distributions. The estimated distribution of plate strength has a mean of 261.47MPa. The predicted distribution tends to overestimate the strength and has a mean of 278.50MPa. Since we consider only one failure mode and limited sources of uncertainty, the overestimation is expected. Despite the difference in the central tendency, the two distributions show very close scatter. The estimated distribution has a standard deviation of 12.12 and the predicted distribution has a standard deviation of 12.09. To achieve the prediction, besides simulations in mesoscale and macroscale, 29 tests in microscale and only 4 tests in mesoscale are performed. This proves that in the proposed framework, with uncertainties propagated from lower scales and limited number of tests in lower scales, an accurate estimation of uncertainty in upper scale can be achieved.
Table 3-1. Test results of 29 T300 single fiber specimens

<table>
<thead>
<tr>
<th></th>
<th>Strain at Tensile strength [mm/mm]</th>
<th>Tensile strength [GPa]</th>
<th>Modulus [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.01381</td>
<td>3.07</td>
<td>202,140.58</td>
</tr>
<tr>
<td>2</td>
<td>0.01242</td>
<td>3.03</td>
<td>220,581.95</td>
</tr>
<tr>
<td>3</td>
<td>0.01330</td>
<td>3.20</td>
<td>216,573.02</td>
</tr>
<tr>
<td>4</td>
<td>0.00878</td>
<td>2.37</td>
<td>214,987.35</td>
</tr>
<tr>
<td>5</td>
<td>0.01141</td>
<td>2.89</td>
<td>200,644.75</td>
</tr>
<tr>
<td>6</td>
<td>0.01519</td>
<td>3.54</td>
<td>200,120.12</td>
</tr>
<tr>
<td>7</td>
<td>0.00867</td>
<td>2.34</td>
<td>201,399.73</td>
</tr>
<tr>
<td>8</td>
<td>0.01144</td>
<td>2.77</td>
<td>227,341.86</td>
</tr>
<tr>
<td>9</td>
<td>0.00780</td>
<td>1.88</td>
<td>220,450.70</td>
</tr>
<tr>
<td>10</td>
<td>0.00753</td>
<td>2.55</td>
<td>205,086.87</td>
</tr>
<tr>
<td>11</td>
<td>0.00793</td>
<td>2.41</td>
<td>219,615.75</td>
</tr>
<tr>
<td>12</td>
<td>0.00578</td>
<td>1.31</td>
<td>187,504.52</td>
</tr>
<tr>
<td>13</td>
<td>0.00831</td>
<td>3.00</td>
<td>221,758.31</td>
</tr>
<tr>
<td>14</td>
<td>0.00401</td>
<td>1.15</td>
<td>185,854.74</td>
</tr>
<tr>
<td>15</td>
<td>0.00679</td>
<td>2.07</td>
<td>203,339.94</td>
</tr>
<tr>
<td>16</td>
<td>0.00654</td>
<td>2.66</td>
<td>205,567.48</td>
</tr>
<tr>
<td>17</td>
<td>0.00450</td>
<td>1.53</td>
<td>214,238.00</td>
</tr>
<tr>
<td>18</td>
<td>0.00540</td>
<td>1.51</td>
<td>192,697.03</td>
</tr>
<tr>
<td>19</td>
<td>0.00563</td>
<td>2.26</td>
<td>206,878.98</td>
</tr>
<tr>
<td>20</td>
<td>0.00438</td>
<td>1.99</td>
<td>216,739.11</td>
</tr>
<tr>
<td>21</td>
<td>0.00551</td>
<td>1.49</td>
<td>202,870.92</td>
</tr>
<tr>
<td>22</td>
<td>0.00353</td>
<td>1.68</td>
<td>213,435.68</td>
</tr>
<tr>
<td>23</td>
<td>0.00475</td>
<td>1.58</td>
<td>198,836.91</td>
</tr>
<tr>
<td>24</td>
<td>0.00550</td>
<td>1.55</td>
<td>206,230.24</td>
</tr>
<tr>
<td>25</td>
<td>0.00701</td>
<td>1.76</td>
<td>207,031.47</td>
</tr>
<tr>
<td>26</td>
<td>0.00526</td>
<td>2.21</td>
<td>192,447.83</td>
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<tr>
<td>27</td>
<td>0.00539</td>
<td>1.74</td>
<td>206,793.66</td>
</tr>
<tr>
<td>28</td>
<td>0.00513</td>
<td>1.93</td>
<td>203,752.26</td>
</tr>
<tr>
<td>29</td>
<td>0.00714</td>
<td>1.71</td>
<td>222,078.46</td>
</tr>
<tr>
<td></td>
<td>Mean</td>
<td>0.00755</td>
<td>2.2</td>
</tr>
<tr>
<td></td>
<td>Standard deviation</td>
<td>0.00317</td>
<td>0.64</td>
</tr>
<tr>
<td></td>
<td>Coefficient of variation</td>
<td>42.02</td>
<td>29.23</td>
</tr>
</tbody>
</table>

Table 3-2. Elastic properties of T300 carbon fiber and PEI

<table>
<thead>
<tr>
<th>T300</th>
<th>$E_{1}$ (GPa)</th>
<th>$E_{2}$ (GPa)</th>
<th>$G_{12}$ (GPa)</th>
<th>$G_{13}$ (GPa)</th>
<th>$v_{12}$</th>
<th>$v_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>207.5</td>
<td>14</td>
<td>9</td>
<td>4</td>
<td>0.2</td>
<td>0.25</td>
</tr>
<tr>
<td>PEI</td>
<td>$E_{m}$ (GPa)</td>
<td>$G_{m}$ (GPa)</td>
<td>$v_{m}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>1.1</td>
<td>0.35</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Table 3-3. Data sheet of Carbon prepreg CF3327

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density of Yarns</td>
<td>count/inch</td>
<td>13</td>
</tr>
<tr>
<td>Fabric Thickness</td>
<td>mm</td>
<td>0.27</td>
</tr>
<tr>
<td>Fabric Areal Weight</td>
<td>g/m²</td>
<td>208.5</td>
</tr>
<tr>
<td>Resin Content</td>
<td>%</td>
<td>37.8</td>
</tr>
</tbody>
</table>

### Table 3-4. Test results of 5 nominally identical specimens

<table>
<thead>
<tr>
<th>Tensile stress at max. load (MPa)</th>
<th>Modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>265.036</td>
<td>12.063</td>
</tr>
<tr>
<td>263.325</td>
<td>12.015</td>
</tr>
<tr>
<td>248.721</td>
<td>13.007</td>
</tr>
<tr>
<td>260.748</td>
<td>12.658</td>
</tr>
<tr>
<td>269.380</td>
<td>12.027</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Tensile stress at max. load (MPa)</th>
<th>Modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>µ</td>
<td>261</td>
</tr>
<tr>
<td>σ</td>
<td>7.775</td>
</tr>
<tr>
<td>CV</td>
<td>2.97%</td>
</tr>
</tbody>
</table>

### Table 3-5. Mean and standard deviation of prior, data and posterior

<table>
<thead>
<tr>
<th></th>
<th>Prior</th>
<th>Data</th>
<th>Posterior</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>383.03</td>
<td>405.69</td>
<td>404.97</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>57.66</td>
<td>31.52</td>
<td>6.84</td>
</tr>
</tbody>
</table>

### Table 3-6. Mean and standard deviation of prior, data and posterior using 4 data

<table>
<thead>
<tr>
<th></th>
<th>Prior</th>
<th>Data</th>
<th>Posterior</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>383.03</td>
<td>373.87</td>
<td>376.00</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>57.66</td>
<td>71.43</td>
<td>16.37</td>
</tr>
</tbody>
</table>
Figure 3-1. Proposed multi-scale uncertainty propagation framework

Figure 3-2. Shape of testing specimen
Figure 3-3. Cutting sides of tab

Figure 3-4. Testing machine. Photos courtesy of author.
Figure 3-5. Histogram of fiber diameters

Figure 3-6. Stress/strain curves of 29 T300 single fiber specimens
Figure 3-7. Histograms of fiber strength and stiffness

Figure 3-8. Comparison of estimated distribution of fiber strength with and without sampling uncertainty
Figure 3-9. Updating fiber volume fraction

\[ V_f = (1 - \alpha \%) \cdot V_{f_0} \]

Figure 3-10. Error of approximation to the standard normal CDF
Figure 3-11. Comparison of developed material subroutine and elastic response in longitudinal direction

Figure 3-12. Effect of mean of fiber strength on yarn strength
Figure 3-13. Effect of coefficient of variation of fiber strength on yarn strength

Figure 3-14. FEA model of prepreg in Abaqus
Figure 3-15. Effect of mean of fiber strength on prepreg strength

Figure 3-16. Effect of coefficient of variation of fiber strength on prepreg strength
Figure 3-17. Specimen of open-hole tension test

Figure 3-18. FEA model of specimen of open-hole tension test
Figure 3-19. Predicted histogram of prepreg strength and test data
Figure 3-20. Posterior of prepreg strength calculated using Bayes’ rule with 18 data
Figure 3-21. Posterior of prepreg strength calculated using Bayes’ rule with 4 data
Figure 3-22. Comparison of estimated distributions using 4 and 18 data with and without prior.
Figure 3-23. Comparison of distribution predicted by surrogate and distribution estimated from test data
CHAPTER 4
CONCLUDING REMARKS

In this dissertation, we first propose a multiscale framework of modeling composites in high strain application. In such an application, fiber breakage is considered as the major failure mode and other progressive failure modes are ignored. Strain rate dependency of mechanical properties of constituents is considered. The proposed framework proves to be accurate compared with test results and a built-in material model of composites in LS-DYNA. And using surrogate modeling technique as constitutive relation offers more flexibility compared with traditional approach of multiscale modeling of composites.

We then move to uncertainty quantification of composites. We propose a multiscale framework to achieve accurate uncertainty quantification of composites. We focus on strength estimation of composites in high strain rate application. In microscale, tests are performed to measure variability of mechanical properties of fiber. In mesoscale, with mechanical properties of fiber and volume fraction as design variables, simulations are performed at different locations to construct a surrogate model to predict prepreg strength. Monte Carlo simulation is employed to provide prior knowledge of the distribution prepreg strength. Then Bayesian inference is used to generate a posterior of prepreg strength to update this knowledge by incorporating test results of prepreg. In macroscale, the above procedures are repeated. Simulations are performed to construct a surrogate model to predict plate strength as a function of prepreg strength. Distribution of plate strength is generated by sampling from posterior of prepreg strength and the built surrogate using Monte Carlo simulation. We show that by propagating uncertainty in lower scale to upper scale and using Bayesian inference to
reduce epistemic uncertainty, we can obtain an accurate estimation of uncertainty in upper scale. In particular, we show that the uncertainty estimation with 29 fiber tests and 4 prepreg tests is more accurate than that of 18 prepreg tests. This can further guide us how to save cost and allocate limited budget among cheap tests in lower scale and expensive tests in upper scale.
APPENDIX
USER-DEFINED MATERIAL SUBROUTINE OF YARN

subroutine vumat(
  C Read only (unmodifiable) variables -
  1  nblock, ndir, nshr, nstatev, nfieldv, nprops, lanneal,
  2  stepTime, totalTime, dt, cmname, coordMp, charLength,
  3  props, density, strainInc, relSpinInc,
  4  tempOld, stretchOld, defgradOld, fieldOld,
  5  stressOld, stateOld, enerInternOld, enerInelasOld,
  6  tempNew, stretchNew, defgradNew, fieldNew,
  C Write only (modifiable) variables -
  7  stressNew, stateNew, enerInternNew, enerInelasNew )
  C
C  include 'vaba_param.inc'
C
    dimension props(nprops), density(nblock), coordMp(nblock,*),
    1  charLength(nblock), strainInc(nblock,ndir+nshr),
    2  relSpinInc(nblock,nshr), tempOld(nblock),
    3  stretchOld(nblock,ndir+nshr), defgradOld(nblock,ndir+nshr+nshr),
    4  fieldOld(nblock,nfieldv), stressOld(nblock,ndir+nshr),
    5  stateOld(nblock,nstatev), enerInternOld(nblock),
    6  enerInelasOld(nblock), tempNew(nblock),
    7  stretchNew(nblock,ndir+nshr), defgradNew(nblock,ndir+nshr+nshr),
    8  fieldNew(nblock,nfieldv), stressNew(nblock,ndir+nshr),
    9  stateNew(nblock,nstatev), enerInternNew(nblock),
    1  enerInelasNew(nblock)
C
    character*80 cmname
C
    double precision EF1, EF2, GF12, GF23, NUF12, NUF23
    double precision EM, GM, NUM, MFSTG, MFST, CVFST, VF0
    double precision F11, F22, F33, F12, F21, F13, F31, F23, F32
    double precision X, Y, S, NCDF, VF
    double precision E1, E2, E3, NU12, NU13, NU23
    double precision G12, G13, G23, NU21, NU31, NU32
    double precision C11, C12, C13, C22, C23, C33
    double precision C44, C55, C66, DELTA
    double precision PI, STRAN(nblock,6)

    parameter(zero = 0.d0, half = 0.5d0, one = 1.d0, two = 2.d0,
    1  PI = 3.14159265359)
C
C  material properties of fiber and matrix
C
EF1 = props(1)
EF2 = 14.0E3
GF12 = 9.0E3
GF23 = 4.0E3
NUF12 = 0.2
NUF23 = 0.25
EM = 3.0E3
GM = 1.1E3
NUM = 0.35

fiber strength

MFSTG = props(2)
MFST = MFSTG/EF1
CVFST = props(3)

initial fiber volume fraction

VF0 = props(4)

elastic constants of yarn calculated by chamis model

E1 = VF0*EF1+(one-VF0)*EM
E2 = EM/(one-SQRT(VF0)*(one-EM/EF2))
E3 = E2
NU12 = VF0*NUF12+(one-VF0)*NUM
NU13 = NU12
G12 = GM/(one-SQRT(VF0)*(one-GM/GF12))
G13 = G12
G23 = GM/(one-SQRT(VF0)*(one-GM/GF23))
NU23 = E2/two/G23-one
NU21 = E2*NU12/E1
NU31 = NU21
NU32 = NU23

stiffness matrix

DELTA = one-NU12*NU21-NU23*NU32-NU13*NU31-two*NU21*NU32*NU13
C11 = (one-NU23*NU32)*E1/DELTA
C22 = (one-NU13*NU31)*E2/DELTA
C33 = (one-NU12*NU21)*E3/DELTA
C12 = (NU12+NU13*NU32)*E2/DELTA
C13 = (NU13+NU12*NU32)*E3/DELTA
C23 = (NU23+NU13*NU21)*E3/DELTA
C44 = G12
C55 = G23
C66 = G13
If stepTime equals to zero, assumes the material pure elastic and use initial elastic modulus

if (stepTime .eq. zero) then
  do i = 1, nblock
    stressNew(i,1)=stressOld(i,1)+C11*strainInc(i,1)
    +C12*strainInc(i,2)+C13*strainInc(i,3)
    stressNew(i,2)=stressOld(i,2)+C12*strainInc(i,1)
    +C22*strainInc(i,2)+C23*strainInc(i,3)
    stressNew(i,3)=stressOld(i,3)+C13*strainInc(i,1)
    +C23*strainInc(i,2)+C33*strainInc(i,3)
    stressNew(i,4)=stressOld(i,4)+two*C44*strainInc(i,4)
    stressNew(i,5)=stressOld(i,5)+two*C55*strainInc(i,5)
    stressNew(i,6)=stressOld(i,6)+two*C66*strainInc(i,6)
  end do
else
  do i = 1, nblock
C
deforation gradient
C
F11=defgradNew(i,1)
F22=defgradNew(i,2)
F33=defgradNew(i,3)
F12=defgradNew(i,4)
F23=defgradNew(i,5)
F31=defgradNew(i,6)
F21=defgradNew(i,7)
F32=defgradNew(i,8)
F13=defgradNew(i,9)
C
eengineering strain
C
STRAN(i,1) = F11-one
STRAN(i,2) = F22-one
STRAN(i,3) = F33-one
STRAN(i,4) = F12+F21
STRAN(i,5) = F23+F32
STRAN(i,6) = F13+F31
C
update fiber volume fraction
C
X = (STRAN(i,1)-MFST)/(CVFST*MFST)
Y = X*X
S = one-(7.0*EXP(-Y/two)+16.0*EXP(-Y*(two-SQRT(two))))
1    +(7.0+PI/4.0*Y)*EXP(-Y))/30.0
NCDF = 0.5+SQRT(S)/two
IF (X .LT. 0.0) NCDF = half-SQRT(S)/two
IF (X .LT. -2.3263) NCDF = zero
IF (X .GT. 2.3263) NCDF = 0.99
VF = VF0*(one-NCDF)
  IF (STRAN(i,1) .GT. 0.013) stateNew(i,1)=0
E1 = VF*EF1+(one-VF0)*EM
C11 = (one-NU23*NU32)*E1/DELTA

C       calculate stress using total strain
C
stressNew(i,1)=C11*STRAN(i,1)+C12*STRAN(i,2)+C13*STRAN(i,3)
stressNew(i,2)=C12*STRAN(i,1)+C22*STRAN(i,2)+C23*STRAN(i,3)
stressNew(i,3)=C13*STRAN(i,1)+C23*STRAN(i,2)+C33*STRAN(i,3)
stressNew(i,4)=C44*STRAN(i,4)
stressNew(i,5)=C55*STRAN(i,5)
stressNew(i,6)=C66*STRAN(i,6)

C       Update the specific internal energy
C
stressPower = half * (  
  1 + ( stressOld(i, 1)+stressNew(i, 1) )*strainInc(i, 1)  
  2 + ( stressOld(i, 2)+stressNew(i, 2) )*strainInc(i, 2)  
  3 + ( stressOld(i, 3)+stressNew(i, 3) )*strainInc(i, 3)  
  4 + two*( stressOld(i, 4)+stressNew(i, 4) )*strainInc(i, 4)  
  5 + two*( stressOld(i, 5)+stressNew(i, 5) )*strainInc(i, 5)  
  6 + two*( stressOld(i, 6)+stressNew(i, 6) )*strainInc(i, 6)  
  )*enerInternNew(i) = enerInternOld(i) + stressPower/density(i)
end do
end if

C       return
end
LIST OF REFERENCES


BIOGRAPHICAL SKETCH

Shu Shang was born in Taikang, China in 1990. He received a Bachelor of Science in mechanical engineering from the Huazhong University of Science and Technology, Wuhan, China in July 2011. For further study, he went to the University of Florida to pursue a master's degree in mechanical engineering and graduated in May 2013. The same year he joined the Structural and Multidisciplinary Optimization Group in University of Florida as a doctoral student under Dr. Nam-Ho Kim. His research interests include: finite element analysis of composites, surrogate and uncertainty quantification.