STRUCTURE GENOME: A REVOLUTIONARY MULTISCALE APPROACH TO BRIDGING MATERIALS GENOME AND STRUCTURAL ANALYSIS

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ABSTRACT

Mechanics of structure genome (MSG) is recently discovered as a formal framework for multiscale constitutive modelling for all composite structures including solids, beams, plates, and shells. MSG is founded on two tenets: the concept of structure genome (SG) and the principle of minimum information loss (PMIL). The basic idea of SG is revisited and further explained and PMIL is formalized in this paper. Its application is demonstrated through constructing models for two well-known problems in composites including computing effective properties of composite laminates and deriving the classical lamination theory.

1 INTRODUCTION

Materials Genome Initiative (MGI) [1], responding to the grand challenges pointed out in the national research council report on Integrated Computational Materials Engineering (ICME) [2], aims to deliver the required infrastructure and training to accelerate discovery, developing, manufacturing, and deploying of advanced materials in a more expeditious and economical way. Because of its potential impact in science and technology, this research started in USA and quickly followed by other parts of the world. Materials modeling advocated by MGI and ICME mainly focuses on the length scale of micron and smaller to link materials behavior with microscopic features and molecular/atomic structures. Optimizing material behavior at this length scale is crucial but should not be the end of the ICME paradigm if these materials are to be used to make materials or structures in larger scales. For example, carbon fiber reinforced composite prepregs are made of carbon fibers (usually a few microns) and resin and have a thickness around 0.1 mm. A composite rotor blade could made of several parts (Skin, Web, D-Spar, etc.) with each part made of dozens or hundreds of composite plies [3]. Ultimately speaking, it is not the material performance, but the structural or system performance we need to optimize. Particularly for composite structures, we expect that MGI and ICME deliver us the properties for the constituents and interfaces between the constituents. These material properties are usually not direct inputs for the structural analysis. Thus, the material modeling in MGI or ICME should be bridged with the macroscopic structural analysis to maximize the benefits of accelerated development of advanced structural materials expected from MGI.

Many systems made of composites such as aircraft, cars, wind turbines, ships, and helicopters are in the size of meters or dozens of meters, structural performance of these systems is significantly affected by their reinforcing fibers in the size of microns. It is computationally impossible to explicitly model fiber details in the system or part level design and analysis. Because at least one element is needed for the fiber, a tiny material block (1 mm³ size) will require a huge computational model with millions of degrees of freedom (DOFs). A normal composite structures will require quadrillions (10¹⁵) of DOFs. It is clearly impractical to design and analyze composite structures through this type of direct numerical simulations (DNS). Instead, we meet this computational challenge using a multiscale approach. Conventional multiscale modelling uses so-called bottom-up approaches. These approaches basically link single-scale models with information passing from smaller scales to larger scales, which can be illustrated using the simple example of analysis of composite laminates made of unidirectional fiber reinforced composites. As shown in Figure 1, a composite laminate is composed of many layers with different fiber directions. The composite layers are made of fiber reinforced composites which
consist of carbon fibers bonded together using a resin material such as epoxy. To avoid capturing the fiber details in the design of the laminate, we first create a unit cell containing two phases: fiber and matrix, with the fiber volume fraction the same as the overall fiber volume fraction in the composite prepreg. Then a micromechanics model is used to replace the original two-phase material with an imaginary homogeneous material with effective properties, the commonly called lamina constants. Many micromechanics based on various assumptions are developed in the literature. Interested readers are referred to [4, 5] for critical evaluations of performances of different micromechanics methods. After this step, the laminate is assumed to be made of homogeneous layers. Even such a model is still too expensive for effective structural design of a system made of composites because each layer should be meshed using multiple 3D solid elements if the finite element analysis (FEA) is used for predicting accurate interlaminar stresses, while the layer thickness is usually very small for typical advanced composite prepregs. One alternative is to use the lamination theory to further eliminate the layerwise details along the thickness direction to obtain a 2D continuum with effective plate/shell properties prescribed for a surface. The final 2D analysis over the reference surface is what is usually used in structural level design and analysis involving composite laminates. For more complex structures, more scales might be involved. For example for a composite stiffened panel made of textile composites. We could have five scales representing fiber, yarn, woven fabric, laminate, and panel. We could compute yarn properties in terms of fiber properties and yarn cross-sectional geometry, then compute woven fabric properties in terms of yarn properties and weave pattern, then compute laminate properties in terms of woven fabric properties, and finally carry out the panel level analysis in terms of the laminate properties.

Usually various assumptions are involved in the model for each scale such as the iso-strain and iso-stress assumptions in rules of mixtures type micromechanics models or Kirchhoff assumptions in the classical lamination theory. The predictive capability of a model greatly depends on the assumptions it invoked in its formulation. Reducing the number of assumptions used in a model will generally increase the accuracy and robustness of the prediction. It is noted that the building block approach extensively used in the aerospace industry also follows the bottom-up multiscale modeling philosophy. Besides the assumptions used in the models for different scales, there is a more fundamental assumption called the scale separation assumption invoked in the bottom-up multiscale modeling. Scale separation assumption is reasonable if the next scale is much larger than the current scale. However, there are many cases for which scale separation is not valid. For example, to analyze a sandwich structure with a honeycomb core, conventional approach will carry out a micromechanical analysis to obtain the core properties first, then analyze the sandwich structure as a laminate made of
homogeneous layers. Significant loss of accuracy will occur even for the global behavior prediction because the size of the honeycomb microstructure is of the same magnitude of the panel thickness and scale separation assumption is not reasonable. Unfortunately these structures are often analyzed using models based on this assumption. Clearly a new multiscale modeling approach is needed to bridge materials with structural analysis avoiding assumptions within each scale and invalid scale assumptions among scales. The recently discovered mechanics of structure genome (MSG) [6] provides a possible answer to this need.

2 MECHANICS OF STRUCTURE GENOME BASED MULTISCALE MODELING

For an engineering structure, despite of its complexity, its mechanical behavior can be modeled by a combination of typical structural components such as solids, plates/shells, beams, and thin-walled beams. If the three dimensions of a component are of similar sizes, it can be modeled as a 3D solid. If one of the dimensions of a component is much smaller than the two other dimensions, it can be modeled as a plate/shell. If two dimensions of a component are much smaller than the third dimension, it can be modeled as a beam. If the sizes of all three dimensions of a component are significantly different from each other, it can be modeled as a thin-walled beam. For each type of the structural components, there is a corresponding structural model governing its behavior. According to continuum mechanics, each structural model contains three sets of equations: kinematics equations, equilibrium equations, and constitutive equations. Both kinematics equations and equilibrium equations can be formulated exactly within the framework of continuum mechanics for linear or nonlinear problems. These two sets of equations remain the same independent of the materials used to make the structure. However, constitutive equations are inherently approximate and different with respect to the material used to make the structure. In the past, constitutive equations for 3D solids are assumed to be of a certain form (e.g. the Hooke’s law) with the material properties measured experimentally. Now, micromechanics is routinely employed to compute 3D properties in terms of microstructural information. Constitutive equations for plates/shells/beams/thin-walled beams are usually derived from the corresponding 3D structural model with some kinematic assumptions such as the famous Euler-Bernoulli assumptions for beams. Such assumptions are usually not valid for composite structures featuring significant anisotropy and heterogeneity at different scales, particularly if the microstructure is important for predicting the corresponding structural behavior.

To circumvent the aforementioned limitations associated with conventional bottom-up multiscale modeling approaches, we prefer a top-down approach by starting from the design and analysis needed for the final structure. As shown in Figure 2, looking at the system, we need to first decide what models we need to capture the behavior relevant to a particular design need. Then we need to decide at which scale we can confidently calibrate our material. Then we need to minimize the information loss between these two model representations of the structure. MSG is what we developed to achieve this purpose [6]. MSG is a formal framework that does not exclusively rely upon direct information passing across scales like conventional bottom-up multiscale modeling approaches, but rather,
operates from the homogenized behavior capturing details at scales relevant to particular design needs. Since we rely on materials modeling of MGI and ICME to link properties of a material with its atomistic/molecular structure, MSG will focus on multiscale modeling for the behavior pertinent to micron scale and larger. Starting from the original model which could be formulated using the 3D continuum mechanics, we need to first identify the structure genome (SG), which is defined as the smallest mathematical building block of the structure. Then we will use the principle of minimum information loss (PMIL) to mathematically decouple the original problem into a constitutive modeling over the SG and a corresponding macroscopic structural analysis. Constitutive modeling over the SG will perform a homogenization analysis to obtain the constitutive models needed for the corresponding macroscopic structural analysis. The macroscopic structural analysis can be routinely carried out using conventional finite element software packages to predict the global behavior which can be used along with the dehomogenization relations from the constitutive modeling to predict the local fields such as stresses and strains within the original structure, which are essential information for more detailed analysis such as the failure analysis.

It is clear that to use MSG-based multiscale modeling we need to answer three fundamental questions for structural modeling. First, what is the macroscopic model wanted for structural design and analysis? The answer to this equation often depends the desired behavior to be captured for a particular design, computing efficiency, and the geometrical characteristics of the structure. Second, what is the original model? The answer to this equation usually depends on the right physics to be captured and it is considered as our truth model. Third, what is the SG? SG is defined as the smallest mathematical building block of the structure. It is the domain for constitutive modeling needed to compute the effective structural properties and perform dehomogenization to predict the local stress and strain fields within the original structure. A different answer to any of these three questions will lead to a different model. Viewing the multiscale modeling from this perspective also provides us the right thinking process for validating our models. The original models should be validated by physical measurements since the major requirement for the original model is to capture the right physics. Right physics is normally known through observations or measurements in labs or the operating environment. The multiscale models we will construct from the original model should be validated by the original model instead. Although many proposed to validate multiscale models using experiments, it is not necessarily the best option. The whole objective of multiscale modeling is to avoid the computational cost of the original model. We can perform a limited number of computationally prohibitive DNS of the original model for the purpose of validating our multiscale models. The answers to the first two questions are relatively straightforward. However, the new concept of SG requires more explanations.

3 STRUCTURE GENOME

Let us first explain SG for slender structures. For example, for design of a composite rotor blade, we are motivated by the slenderness of the structure to use a beam model such as the Euler-Bernoulli model or the Timoshenko model to simplify our analysis. The chosen beam model will be our macroscopic model we want to construct for the rotor blade. If we focus on the elastic behavior and if we assume each composite layer is a homogeneous anisotropic material, the original model of a composite rotor blade is the 3D anisotropic elasticity theory with layerwise heterogeneities. The SG of the structure is the cross-section if the composite blade can be
approximated as made of a uniform cross-section or an assembly of segments made of a uniform cross-section for each segment. A constitutive modeling over the cross-section will predict the equivalent beam properties for the 1D beam analysis and also provide dehomogenization relations to recover the local stress/strain field within the original 3D structure. As shown in Figure 3, if we want to model the elastic behavior of slender structures with spanwise heterogeneity using the same beam model, we only need to change the answer to the third question to be a 3D block containing the corresponding heterogeneity. Furthermore, changing the answer to the first question will also enlarge the application domain. For example, if we change the original model to be 3D anisotropic elasticity theory with possible pointwise heterogeneities, then we have the possibility to directly compute equivalent beam properties in terms of fiber/matrix properties and recover stress/strain fields at the fiber/matrix level.

If we want to construct models for panels (structures with one of its dimensions much smaller than the other two dimensions), the answer to the first question will be a corresponding plate or shell model such as Kirchhoff-Love model or Reissner-Mindlin model. The corresponding SG (the answer to the third equation) can be chosen based on the internal construction of the panel as shown in Figure 4. If the panel can be assumed as a laminate made of homogeneous layers, the SG will be the 1D transverse normal line. If the panel has heterogeneity in one of its in-plane directions, the SG will be a 2D domain. If the panel has heterogeneity in both in-plane directions, the SG will be a 3D block. Despite of the SG dimensionalities, a constitutive modeling over the SG will predict the equivalent plate/shell properties for the corresponding plate/shell model (e.g. Kirchhoff-Love model or Reissner-Mindlin model) used in the 2D plate/shell analysis and also provide dehomogenization relations to predict the local stress/strain field within the original 3D structure.

If we want to construct models for structures with all three dimensions having similar size (see Figure 5), the answer to the first question will be a corresponding solid model such as the 3D elasticity model. The corresponding SG can be chosen based on the internal construction of the structure. For 3D structures, SG serves a similar role as representative volume element (RVE) in micromechanics. However, they are significantly different. For example, for a structure made of composites featuring 1D heterogeneity (e.g. binary composites made of two alternating layers, Figure 5a), the SG will be a straight line with two segments denoting corresponding phases. Another
possible application is to model a laminate as an equivalent homogeneous solid. The transverse normal line is the 1D SG for the laminate. The constitutive modeling over the 1D SG can be used to compute the complete set of 3D properties and local fields. Such applications of SG are not equivalent to RVE. For a structure made of composites featuring 2D heterogeneity (e.g. continuous unidirectional fiber reinforced composites, Figure 5b), the SG will be a 2D domain. Although 2D RVEs are also used, only in-plane properties and local fields can be obtained from common RVE-based models. If the complete set of properties are needed for a 3D structural analysis, a 3D RVE is usually required [7], while a 2D domain is sufficient if it is modeled using SG-based models. For a structure made of composites featuring 3D heterogeneity (e.g. particle reinforced composites, Figure 5c), the SG will be a 3D volume. It is clear that the SG concept, when applied to 3D structures, essentially provides a general theory for constructing micromechanics model for all types of heterogeneous microstructures.

The SG concept also sheds new insights into structural modeling for beams, plates, and shells. If we consider the reference line for a beam or the reference surface for a plate/shell as a generalized continuum, every material point of this continuum has a microstructure which is the SG. A homogenization over the SG will compute the effective (structural) properties for the macroscopic analysis of the continuum and a dehomogenization over the SG will compute the local fields. In other words, structural modeling for beams/plates/shells becomes a special application of micromechanics. Unlike the conventional notation of beams, plates, or shells, the SG concept also provides a systematic way to construct a beam/plate/shell model for any structure with or without heterogeneities that the user wants to model it as a beam, plate, or shell.

It is easy to identify SGs for periodic structures as shown in Figures 3, 4, 5. Real composite structures are usually not periodic. We often assume that the structure is at least periodic in the neighborhood of a material point in the macroscopic structural analysis, the so-called local periodicity assumption implicit in all multiscale modeling approaches [8]. For nonlinear behavior, it is also possible that the smallest mathematical building block of the structure is not sufficient as the characteristic length scale of the nonlinear behavior may cover several building blocks. For this case, SG should be interpreted as the smallest mathematical building block necessary to represent the nonlinear behavior. For most general cases, SG can be considered as the block of material corresponding to the element in the macroscopic structural analysis. A structure could have as many SGs as the number of elements in the macroscopic structural analysis.

4 PRINCIPLE OF MINIMUM INFORMATION LOSS

The principle of minimum information loss (PMIL) is used to formulate MSG. Specifically, PMIL states that the macroscopic model can be constructed from the original model by minimizing the difference of information of the original model and the macroscopic model. We need to decide what will be the information measure necessary to describe the original model. Then we need to express the information of the original model in terms of field variables of the macroscopic model and some unknown functions. These unknown functions can be solved by minimizing the difference of the information of the original model and that of the macroscopic model. Let us illustrate the basic idea of PMIL using elastic behavior of a structure. For this case, the strain energy will be a natural choice as the information measure because the elastic constitutive behavior is governed by the strain energy.

First, we need to express the displacement fields of the original model (\(\mathbf{u}\)) in terms of that of the macroscopic model (\(\mathbf{\bar{u}}\)) and some unknown functions (\(\chi\)). These unknown functions are called warping functions in structural mechanics, and fluctuating functions in micromechanics. In MSG, they are called fluctuating functions for simplicity because structural modeling is a special application of microstructure due to the SG concept. These relations can be symbolically written as

\[
\mathbf{u} = \mathbf{u}(\mathbf{\bar{u}}, \chi)
\]

Then based on the strain definition of the original model and the strain definition of the macroscopic model, we can derive the following relations to relate these two sets of strain variables:

\[
\mathbf{\varepsilon} = \mathbf{\varepsilon}(\mathbf{\bar{\varepsilon}}, \nabla \chi)
\]

It is noted that these two sets of strains could be defined differently based on the choice of the original model and the macroscopic model. Since we are constructing the macroscopic model out of the
original model, we consider that the original model is true and we need to define the kinematic fields (including both the displacements and strains) of the macroscopic model in terms those of the original model, which will effectively introduce constraints on the fluctuating functions.

If we choose the strain energy as the information governing the constitutive relations for the physical behavior we are after, we can express the strain energy of the original model as

$$ U = U(\varepsilon, \nabla \chi) $$

To minimize the loss of information, the strain energy in this case, between original model and the macroscopic model, we can establish the following variational statement over the SG

$$ \min_{\chi} U(\varepsilon, \nabla \chi) - \tilde{U}(\varepsilon) $$

subject to the constraints on $\chi$ previously introduced due to the kinematic equivalence and due to other considerations such as periodic feature of the SG along certain directions. This variational statement can be straightforwardly solved using a numerical technique such as the finite element method. Note here we only used the strain energy for illustrative purpose. The information governing the original model and the macroscopic model can also be potential energy, virtual work, dissipation, etc depending on the physics to be captured. Even we only focus on the strain energy, there are many problems MSG can be used to solve, which will be shown in the next section.

5 SAMPLE APPLICATIONS OF MSG

In this section, we will illustrate the application of MSG to a few well known problems in mechanics of composites including computing effective properties of composite laminates and deriving the classical lamination theory.

5.1 Compute effective properties of composite laminates

In practice, effective laminate properties are often needed for efficient design and analysis. In-plane properties can be easily obtained using CLT. However, it is not easy to obtain through-the-thickness properties and many different set of assumptions are introduced to achieve this purpose [9]. We will show how one can use MSG to solve this problem. As shown in Figure 6, according to MSG, we know the original model is 3D continuum mechanics with layerwise heterogeneity with each layer assumed to be homogeneous and anisotropic. The macroscopic model is 3D continuum mechanics with homogeneity through the thickness, which is also commonly called as a black aluminum. The SG is the transverse normal line.

We first express the displacements of the original model in terms of that of the macroscopic model and unknown fluctuating functions such that

$$ u_i = \bar{u}_i + \chi_i $$

Then we can obtain the strain field of the original model in terms of the macroscopic model as

$$ \varepsilon_{ij} = \bar{\varepsilon}_{ij} + \frac{1}{2}(\chi_{i,j} + \chi_{j,i}) $$

Figure 6. Computing effective properties of composite laminates using MSG.
We can define the displacement and strain fields of the macroscopic model to be the same as the average of the corresponding fields of the original model over the thickness, which results in the following constraints on the fluctuating functions:

\[ \langle \chi_i \rangle = 0 \quad \langle \chi_{ij} + \chi_{ji} \rangle = 0 \]  

Using Eq. (6), we can express the strain energy of the original model as

\[ U = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} = \frac{1}{2} C_{ijkl} (\bar{\varepsilon}_{ij} + \chi_{ij}) (\bar{\varepsilon}_{kl} + \chi_{kl}) \]  

PMIL can be written as

\[ \min \left\{ \frac{1}{2} C_{ijkl} (\bar{\varepsilon}_{ij} + \chi_{ij}) (\bar{\varepsilon}_{kl} + \chi_{kl}) - \frac{1}{2} C_{ijkl}^* \bar{\varepsilon}_{ij} \bar{\varepsilon}_{kl} \right\} \]  

which can be used to solve for \( \chi_i \). Since it is a 1D problem, the exact solution can be obtained analytically. We find out that according to this solution, the in-plane strains and transverse stresses must be constant through the thickness. These facts can be used to easily compute the complete set of effective properties of the composite laminates. For more details, interested readers are referred to [10].

It is clear that MSG enables us to formulate the problem in a systematic way and obtain the exact solution within the premise of the problem itself without introducing apriori assumptions as done by other approaches in the literature [10].

5.2 Deriving the classical lamination theory

CLT is often used for design and analysis related with composite laminates and its derivation are covered in all textbooks on composite mechanics. Traditionally, the plane-stress assumption is first introduced to obtain the plane-stress reduced constitutive relations for each lamina, then Kirchhoff assumptions (transverse normal remains straight, normal, and rigid) are used to express displacements and strains in terms of plate displacements and strains [11]. Although often neglected, there is a blatant contradiction between the plane-stress assumptions and Kirchhoff assumptions because it is impossible, even for isotropic plates, for the transverse normal to not deform along the thickness direction yet remain a plane-stress state, unless the Poisson’s ratio is zero. We will show how one can use MSG to derive the CLT without introducing such conflicting assumptions. As shown in Figure 7, according to MSG, we know that the original model is 3D continuum mechanics with layerwise heterogeneity and each layer assumed to be homogeneous and anisotropic. The macroscopic model is a 2D plate model. The SG is the transverse normal line. It is interesting to know that comparing to the problem of computing effective 3D properties for composite laminate, among the answers to three fundamental questions needed for MSG-based multiscale modeling, only the macroscopic model is different and both the original model and SG remain the same.

According to MSG, we first express the displacements of the original model in terms of that of the plate model and unknown fluctuating functions such that
\[ u_1(x_1, x_2, x_3) = \bar{u}_1(x_1, x_2) - x_3 \bar{\alpha}_1(x_1, x_2) + \chi_1(x_1, x_2, x_3) \]
\[ u_2(x_1, x_2, x_3) = \bar{u}_2(x_1, x_2) - x_3 \bar{\alpha}_2(x_1, x_2) + \chi_2(x_1, x_2, x_3) \]
\[ u_3(x_1, x_2, x_3) = \bar{u}_3(x_1, x_2) + \chi_3(x_1, x_2, x_3) \]

Then we can obtain the strain field of the original model in terms of the plate model as
\[ e_{11} = \bar{e}_{11} + x_3 k_{11} \]
\[ e_{22} = \bar{e}_{22} + x_3 k_{22} \]
\[ 2e_{12} = \bar{e}_{12} + 2x_3 k_{12} \]
\[ 2e_{13} = \chi_{1,3} \]
\[ 2e_{23} = \chi_{2,3} \]
\[ e_{33} = \chi_{3,3} \]

We can define the displacements of the plate model to be the same as the average of the corresponding fields of the original model over the thickness, which results in the following constraints on the fluctuating functions:
\[ \langle \chi_i \rangle = 0 \]

Using Eq. (11), we can express the strain energy of the original model as
\[ U = \frac{1}{2} C_{ijkl} e_{ij} e_{kl} \]

PMIL can be written as
\[ \min_{\chi} \frac{1}{2} C_{ijkl} e_{ij} e_{kl} - \frac{1}{2} \left[ e \right]^T \left[ A \ B \right] \left[ e \right] - \frac{1}{2} \left[ k \right]^T \left[ B \ D \right] \left[ k \right] \]

which can be used to solve for \( \chi_i \). Since it is a 1D problem, the exact solution can be obtained analytically. We find out that according to this solution, the transverse stresses must vanish. In other words, the plane-stress assumption we used to derive CLT in the traditional way is valid. However, the transverse normal is not rigid, both transverse normal and shear strains could exist. It is clear that MSG enables us to formulate the problem in a systematic way and obtain the exact solution within the premise of the problem itself without introducing apriori assumptions as done by other approaches in the literature [11].

5 CONCLUSION

A novel multiscale modelling framework is proposed based on the recently discovered mechanics of structure genome (MSG). The concept of structure genome (SG) is explained in details and the principle of minimum information loss (PMIL) is formalized as a general principle to construct models for composite structures and materials. The application of MSG is demonstrated through solving two well-known problems in composites including computing effective properties of composite laminates and deriving the classical lamination theory. It is clear that MSG provides a systematic framework for composites modelling without invoking assumptions within each scales and invalid scale separation assumptions among scales. After identifying the answers to three fundamental questions: what is the original model, what is the macroscopic model, and what is the SG, PMIL is used to construct the best macroscopic model out of the original model. We have also demonstrated its application to slender structures [12] and free-edge stresses [13], textile composites [14]. In principle, MSG provides a general, unified framework for constructing models for all types of composite structures as long as the original model and the corresponding SG can be identified. Many more applications of this versatile modelling framework are yet to be discovered.

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