### SwiftComp<sup>TM</sup> User Manual

Version 1.4

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### 1 Introduction

SwiftComp<sup>TM</sup> represents a general-purpose computational approach for constitutive modeling of composite materials and structures. Here composite materials and structures refer to those materials and structures featuring anisotropy and heterogeneity, not just the traditional notion of fiber reinforced polymers. It can be used independently as a tool for virtual testing of composite materials and structures or as a plugin to power conventional finite element analysis (FEA) codes with efficient high-fidelity multiscale modeling for such materials and structures. SwiftComp<sup>TM</sup> implements Mechanics of Structure Genome (MSG), a unique multiscale modeling approach based on the concept of Structure Genome (SG), which assures the best accuracy at the speed of engineering design to capture both anisotropy and heterogeneity of composites at the microscopic scale or other scales of user's interest. MSG unifies micromechanics and structural mechanics to provide a single approach to model all types of composite materials and structures. SwiftComp<sup>TM</sup> enables engineers to model composites similarly to metals, capturing details as needed and affordable.

To facilitate the use of SwiftComp<sup>TM</sup>, several graphic user interfaces have been developed including Gmsh4SC, TexGen4SC, ABAQUS-SwiftComp GUI, and ANSYS-SwiftComp GUI. How to use SwiftComp<sup>TM</sup> through these GUIs has been given in user manuals accompanying the corresponding GUIs. This manual will provide an introduction to MSG, the history and functionalities of SwiftComp<sup>TM</sup>, conventions, inputs, outputs, maintenance, and tech support.

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## ${\bf 2}\quad {\bf SwiftComp}^{\rm TM}\ {\bf History}$

SwiftComp<sup>TM</sup> is a culmination of prior work on composite structures and materials implemented in three different codes including VABS, VAPAS, and VAMUCH developed by Prof. Wenbin Yu and his coworkers. The VABS code was developed for composite beam modeling during Prof. Yu's PhD study at Georgia Tech under the supervision of Prof. Dewey Hodges. VABS was later significantly enhanced at Utah State through its affiliation with Georgia Tech's rotorcraft center and commercialized by Utah State through AnalySwift LLC. Prof. Yu also developed VAPAS to model composite plates & shells at Georgia Tech and VAPAS was also later enhanced at Utah State. VAMUCH, also called SwiftComp Micromechanics<sup>TM</sup>, is a general-purpose micromechanics code for homogenization and dehomogenization of periodic, heterogeneous materials developed at Utah State University. In year 2012, Prof. Yu introduced the representative structural element (RSE) concept to unify structural mechanics and micromechanics for multiscale constitutive modeling of composites [1]. RSE concept was later renamed as SG to emphasize its role in filling the gap between materials genome and structural analysis [2]. The funding paper of MSG was published in year 2016 [3]. To implement MSG, we started the development of SwiftComp<sup>TM</sup> in April 2014 at Purdue University. SwiftComp<sup>TM</sup> is a single code which can reproduce all the functionalities in VABS, VAPAS, and VAMUCH, as well as many other capabilities not found in any of those three codes. SwiftComp<sup>TM</sup> can reproduce VABS for composite beams made of uniform cross-section (see the right figure of Figure 4), VAPAS for composite plates/shells made of homogeneous layers (see the right figure of Figure 5), and VAMUCH for 3D periodic heterogeneous materials and structures (see Figure 3). However, currently not all VABS capabilities are available in SwiftComp<sup>TM</sup> and VABS is still kept maintained as a separate code for cross-sectional analysis of composite beams. SwiftComp<sup>TM</sup> has many more functionalities not available in the previous three codes such as slender structures with spanwise heterogeneities, plates/shells with in-plane heterogeneity, partially periodic structures and materials, aperiodic structures and materials, etc.

### 3 SwiftComp<sup>TM</sup> Functionalities

Fundamentally speaking, SwiftComp<sup>TM</sup> takes the geometry and material characteristics of an SG described using a finite element mesh as the input and computes the effective properties for the macroscopic analysis. This process is commonly called *homogenization*. SwiftComp<sup>TM</sup> can also compute the local fields within the SG based on global behavior obtained from the macroscopic analysis. This process is commonly called *dehomogenization*, constantly neglected in some multiscale modeling approaches. Note that SwiftComp<sup>TM</sup> is not limited to structural modeling, it can be used to perform multiphysics homogenization and dehomogenization of materials and structures responsive to thermal, mechanical, electric, and magnetic fields.

### 3.1 Alpha Version

The alpha version of SwiftComp<sup>TM</sup> can perform the constitutive modeling corresponding to the classical structural models including the Euler-Bernoulli beam model, Kirchhoff-Love plate/shell model, and 3D Cauchy continuum model.

### 3.2 Version 1.0

Starting SwiftComp<sup>TM</sup> 1.0, two versions of SwiftComp<sup>TM</sup> is possible: SwiftComp<sup>TM</sup> Standard and SwiftComp<sup>TM</sup> Professional. In SwiftComp<sup>TM</sup> Professional, a direct sparse solver is used to deal with big models which could have as many as millions of degrees of freedom. A parallel edition is also available for SwiftComp<sup>TM</sup> Professional. For a problem that SwiftComp<sup>TM</sup> Professional runs more than a few minutes, it is better to use the parallel edition as it can exploit multiple cores which are readily available on most computers nowadays. In the standard version, Prof. Sloan's method<sup>4</sup> is used to provide the renumbering of the finite element mesh, standard skyline storage is used along with a regular direct linear solver. To simplify the maintenance of the code, the later official released version is the parallel version with direct sparse solver.

#### 3.2.1 Version 1.1

The pointwise anisotropic heterogeneity is enabled in SwiftComp<sup>TM</sup> 1.1. The SG can contain phases with general anisotropic materials with material properties given in material coordinates which could be different from the local coordinate system and defined for each element. First, an elemental coordinate system is defined by three points for each element, then the material coordinate system can be defined as a simple rotation around one of the axis of the elemental coordinate element.

#### 3.2.2 Version 1.2

SwiftComp<sup>TM</sup> 1.2 implements the capability to deal with aperiodic, or partially periodic SGs, or periodic SGs without periodic nodes on the boundary surfaces.

#### 3.2.3 Version 1.3

SwiftComp<sup>TM</sup> 1.3 implements the capability to predict initial failure strengths according to a given failure criterion, failure envelopes for giving two load directions, and failure indexes and strength ratios for the material subject to an arbitrary loading.

#### 3.2.4 Version 1.4

SwiftComp<sup>TM</sup> 1.4 implements homogenization, dehomogenization, initial failure analysis accorading to the Timoshenko beam model.

### 4 Structures and Structural Models

To understand the meaning of SG, we need to define what is a structure. Structure and material often appear together and sometimes are used interchangeably. The main reason is that the difference between structure and material is not clear. The interchangeable use of these two terms starts from the first solid mechanics course, usually called either *Strength of Materials* or *Mechanics of Materials*, mainly covers stress analysis of various structures including rods, shafts, columns, beams, pressure vessels, etc. With the extensive penetration of composites in industry and the increasing

capabilities of fabricating materials with complex microstructures, the difference between structure and material becomes even more elusive.

One possible differentiator is the presence of boundary: the material itself has no boundaries, but rather may be considered as a point in a structure according to the continuum hypothesis. Another differentiator is that we describe a material using material properties such as Young's moduli, Poisson's ratios, coefficients of thermal expansion (CTEs), yielding limits, ultimate strengths, etc. These properties are intrinsic to the material, and will not change for different structures which could be made of the same material. For example, if a linear elastic material has Young's modulus equal to 73 GPa, it will always remain this value no matter whether it is used to make a shaft or a pressure vessel, subject to a force of 10 N or 10 kN. It is noted that for nonlinear behavior, the material properties could depend on the current stress or strain state which the material is experiencing but these properties are genetic (or intrinsic) to the material which means even if the material is not experiencing any stress or strain right now, the same constitutive relations exist.

On the other hand, a structure is a solid body made of one or more materials with clearly defined interactions with its external environment through boundary conditions, applied loads, and environment effects, e.q., temperature, moisture, etc. The behavior of a structure is usually described using displacements, strains, stresses, natural frequencies, buckling loads, and failure. Structures can be categorized in terms of its external geometry. If the three dimensions of a structure are of similar size, it is called a 3D structure (Figure 1 a). If one dimension of the structure is much smaller than the two other dimensions, the structure is called as a plate (Figure 1 b) or shell (Figure 1 c) depending on whether it is flat or curved along the two large dimensions. Usually the small dimension is called thickness and the two large dimensions are called the in-plane directions. A reference surface can be defined for a plate or shell using the two in-plane coordinates. If one dimension of the structure is much larger than two other dimensions, the structure is called as a beam (Figure 1 d). Usually the large dimension is called the length, span, or axis of the beam and a reference line can be defined for a beam using the axial coordinate. The reference line can be as general as a spatial curve which is the case for initially curved and twisted beams. The two small dimensions are commonly called the cross section for typical beam-like structures. As far as the mathematical modeling is concerned, this classification only considers the external geometry and the internal construction of these structures can be arbitrary. For example, a porous material with holes in the body can be modeled as a 3D solid, a sandwich flat panel with a honeycomb core can be modeled as a plate, a high aspect ratio wing of aircraft can be modeled as a beam with no clearly defined cross sections. In this sense, all engineering structural systems, despite its complexity, can be considered as formed by using a combination of structural components in terms of 3D structures, plates/shells, and/or beams as shown in Figure 1 with possible complex internal constructions.

How to predict displacements, strains, and stresses within structures using mathematical models belongs to a long standing branch of applied mechanics call structural mechanics. Although there are historical and practical reasons for classifying structures as 3D structures, plates/shells, and beams, different names for different structures have also motivated us to construct different mathematical models for the analyses of corresponding structures. Let us use  $x_1, x_2, x_3$  denotes the global Cartesian coordinate system. Beams, plates, shells are also collectively called dimensionally

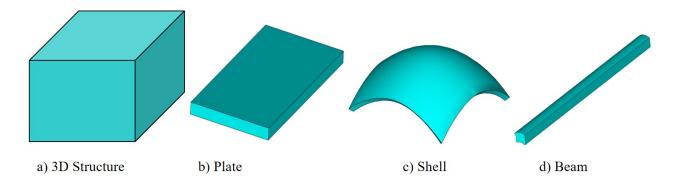


Figure 1: Typical structural components.

reducible structures because it is possible for us to eliminate the small dimension(s) to create dimensionally reduced models for these structures [5]. More specifically, we can create one-dimensional (1D) structural models (also called beam models) of which the field variables are functions of  $x_1$ , the coordinate describing the beam reference line, for beam-like structures. We can also create two-dimensional (2D) structural models (also called plate/shell models) of which the field variables are functions of  $x_1$  and  $x_2$ , the two in-plane coordinates, for plate/shell-like structures. Here, the notation of 1D, 2D, or 3D refers to the number of coordinates needed to describe the analysis domain. It does not correspond to the dimensionality of the behavior. For example, a 1D beam model can describe the deformation and rotation of the structure in all the three directions in space. Each model contains three sets of equations including kinematics, kinetics, and constitutive relations, among which only the constitutive relations change for different materials used to make the structure. For composites, the stiffness matrix could be fully populated. The task to predict the constitutive models is called *constitutive modeling*. 3D properties in terms of Young's moduli, Poisson's ratios, and shear moduli, could be obtained either experimentally or through a micromechanics calculation. For isotropic homogeneous structures, 3D material properties are direct inputs for structural analysis using a 3D solid model, and these properties combined with geometric characteristics of the structure can be used for structural analysis using plate/shell/beam models with the structural stiffness (e.q., EA, EI, GJ) obtained based on apriori assumptions such as the Euler-Bernoulli assumptions for beams. However, such straightforwardness does not exist for structures featuring anisotropy and/or heterogeneity. Many refined assumptions, such as higher-order assumptions, zigzag assumptions, layerwise assumptions, have been introduced to better capture the kinematics along the smaller dimensions of the structure, e.g. the thickness of a plate/shell, or the cross section of a beam in other approaches.

Structural analyses are routinely carried out using the finite element analysis (FEA) codes such as ABAQUS, ANSYS, and NASTRAN in terms of 3D solid elements, 2D plate or shell elements, or 1D beam elements (see Figure 2). Each element type is governed by a corresponding structural model which contains kinematics, kinetics, and constitutive relations. The commonly used beam models in engineering include the Euler-Bernoulli model, and the Timoshenko model. The Euler-Bernoulli model is also commonly called the classical beam model. The commonly used plate/shell models in engineering are the Kirchhoff-Love model, and the Reissner-Mindlin model.

The Kirchhoff-Love model is also commonly called the classical plate/shell model. The commonly used 3D model in engineering is the Cauchy continuum model which is also commonly called the classical continuum model. Here, we will restrict ourselves to structures made of linear elastic materials to illustrate the basics of each structural model although it is emphasized that MSG has no such restriction. The models for structures featuring geometrical and material nonlinearities can be found in relevant MSG publications.

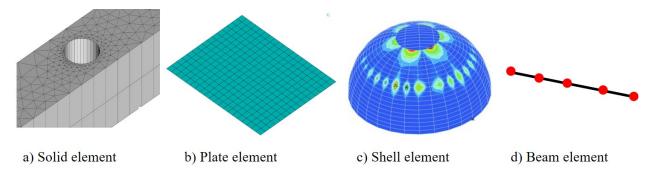


Figure 2: Typical structural elements.

### 4.1 3D Cauchy Continuum Model

The kinematics of the Cauchy continuum model contains three displacements  $u_1, u_2, u_3$  and six strains  $\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \varepsilon_{23}, \varepsilon_{13}, \varepsilon_{12}$  which are all functions of three coordinates  $x_1, x_2, x_3$ . For this very reason, it is called a 3D model. The strain-displacement relations are given as

$$\varepsilon_{11} = \frac{\partial u_1}{\partial x_1} \quad \varepsilon_{22} = \frac{\partial u_2}{\partial x_2} \quad \varepsilon_{33} = \frac{\partial u_3}{\partial x_3} 
2\varepsilon_{23} = \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \quad 2\varepsilon_{13} = \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \quad 2\varepsilon_{12} = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}$$
(1)

The kinetics of the Cauchy continuum model is described using six stresses  $\sigma_{11}$ ,  $\sigma_{22}$ ,  $\sigma_{33}$ ,  $\sigma_{23}$ ,  $\sigma_{13}$ ,  $\sigma_{12}$  which are all functions of  $x_1, x_2, x_3$ . These stresses are governed by the following equations of equilibrium.

$$\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} + \frac{\partial \sigma_{13}}{\partial x_3} + f_1 = 0$$

$$\frac{\partial \sigma_{12}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \sigma_{23}}{\partial x_3} + f_2 = 0$$

$$\frac{\partial \sigma_{13}}{\partial x_1} + \frac{\partial \sigma_{23}}{\partial x_2} + \frac{\partial \sigma_{33}}{\partial x_3} + f_3 = 0$$
(2)

where  $f_1, f_2, f_3$  are distributed body forces. The constitutive relations of the Cauchy continuum model for the linear elastic behavior are described using the generalized Hooke's law as

$$\begin{cases}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{23} \\
\sigma_{13} \\
\sigma_{12}
\end{cases} = \begin{bmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\
C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\
C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\
C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66}
\end{bmatrix} \begin{pmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
2\varepsilon_{23} \\
2\varepsilon_{13} \\
2\varepsilon_{12}
\end{cases}$$
(3)

The  $6 \times 6$  matrix  $C_{ij}$  is called the stiffness matrix and its inverse is called the compliance matrix. Note that material properties are usually provided in the so-called material coordinate system which implies that we need to write constitutive relations in the material coordinate system first. However, the kinematics and kinetics are usually formulated in the global coordinate system. A proper transformation according to the tensorial transformation laws is needed to transfer the constitutive relations into the global coordinate system.

For isotropic materials, the constitutive relations can be expressed in terms of the Young's modulus E and Poisson's ratio  $\nu$  as

$$\begin{cases}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
2\varepsilon_{23} \\
2\varepsilon_{13} \\
2\varepsilon_{12}
\end{cases} = \begin{bmatrix}
\frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\
-\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\
-\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{2(1+\nu)}{E} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{2(1+\nu)}{E} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{2(1+\nu)}{E}
\end{cases} \begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{23} \\
\sigma_{13} \\
\sigma_{12}
\end{cases}$$
(4)

which can be inverted to obtain the same expression as Eq. (3) with

$$C_{11} = C_{22} = C_{33} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}$$

$$C_{12} = C_{13} = C_{23} = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

$$C_{44} = C_{55} = C_{66} = \frac{E}{2(1+\nu)}$$

and all other terms in the stiffness matrix of Eq. (3) are zero.

For orthotropic materials, the constitutive relations can also be expressed as

$$\begin{cases}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
2\varepsilon_{23} \\
2\varepsilon_{13} \\
2\varepsilon_{12}
\end{cases} = \begin{bmatrix}
\frac{1}{E_1} & -\frac{\nu_{21}}{E_2} & -\frac{\nu_{31}}{E_3} & 0 & 0 & 0 \\
-\frac{\nu_{12}}{E_1} & \frac{1}{E_2} & -\frac{\nu_{32}}{E_3} & 0 & 0 & 0 \\
-\frac{\nu_{13}}{E_1} & -\frac{\nu_{23}}{E_2} & \frac{1}{E_3} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{G_{23}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{G_{13}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{G_{13}}
\end{cases} \begin{cases}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{23} \\
\sigma_{13} \\
\sigma_{12}
\end{cases}$$
(5)

where  $E_1, E_2, E_3$  are Young's moduli in three directions,  $G_{12}, G_{13}, G_{23}$  are shear moduli in three directions,  $\nu_{12}, \nu_{13}, \nu_{23}$  and  $\nu_{21}, \nu_{31}, \nu_{32}$  are two set of Poisson's ratios. Usually only  $\nu_{12}, \nu_{13}, \nu_{23}$  are given and the other Poisson's ratios are calculated as

$$\nu_{21} = \nu_{12}E_2/E_1$$
  $\nu_{31} = \nu_{13}E_3/E_1$   $\nu_{32} = \nu_{23}E_3/E_2$ 

due to the symmetry of the compliance matrix.

Eq. (5) can be inverted to obtain the same expression as Eq. (3) with

$$C_{11} = E_1(1 - \nu_{23}\nu_{32})/\Delta \qquad C_{12} = E_2(\nu_{12} + \nu_{13}\nu_{32})/\Delta \qquad C_{13} = E_3(\nu_{13} + \nu_{12}\nu_{23})/\Delta$$

$$C_{22} = E_2(1 - \nu_{13}\nu_{31})/\Delta \qquad C_{23} = E_3(\nu_{23} + \nu_{13}\nu_{21})/\Delta \qquad C_{33} = E_3(1 - \nu_{12}\nu_{21})/\Delta$$

$$C_{44} = G_{23} \qquad C_{55} = G_{13} \qquad C_{66} = G_{12}$$

with

$$\Delta = 1 - \nu_{12}\nu_{21} - \nu_{23}\nu_{32} - \nu_{13}\nu_{31} - 2\nu_{21}\nu_{13}\nu_{32}$$

and all other terms in Eq. (3) are zero.

Eqs. (1), (2), and (3) form a system of 15 equations underpinning the Cauchy continuum model to be solved along with appropriate boundary conditions for 15 unknowns (3 displacements, 6 strains, and 6 stresses). This model has been implemented in many FEA codes which have 3D solid elements. Kinematics and kinetics remain the same no matter whether the structure is made of metals or composites. Only difference is in the constitutive relations, see Eq. (3) for general anisotropic materials, Eq. (4) for isotropic materials, and Eq. (5) for orthotropic materials.

It is worthy to point out that there are two degenerated version of the 3D Cauchy continuum model: plane stress model and plane strain model. Plane stress model assumes that all the out-of-plane stresses vanish. For example, if the plane stress model is formulated in the  $x_1 - x_2$  plane, we assume  $\sigma_{13} = \sigma_{23} = \sigma_{33} = 0$ . Plane strain model assumes that all the out-of-plane strains vanish. For example, if the plane strain model is formulated in the  $x_1 - x_2$  plane, we assume  $\varepsilon_{13} = \varepsilon_{23} = \varepsilon_{33} = 0$ . The kinematics of the plane stress model and plane strain model remain the same as

$$\varepsilon_{11} = \frac{\partial u_1}{\partial x_1} \qquad \varepsilon_{22} = \frac{\partial u_2}{\partial x_2} \qquad 2\varepsilon_{12} = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \tag{6}$$

The kinetics of the plane stress model and plane strain model remain the same as

$$\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{12}}{\partial x_2} + f_1 = 0$$

$$\frac{\partial \sigma_{12}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} + f_2 = 0$$
(7)

The constitutive relations of the plane strain model are

The constitutive relations of the plane stress model are

where  $Q_{ij}$  are the so-called plane-stress-reduced stiffnesses which are different from  $c_{ij}$ . They are computed by substituting  $\sigma_{13} = \sigma_{23} = \sigma_{33} = 0$  into Eq. (3) to obtain  $\varepsilon_{33}, 2\varepsilon_{23}, 2\varepsilon_{13}$  in terms of  $\varepsilon_{11}, \varepsilon_{22}, 2\varepsilon_{12}$ . Then substituting these relations back into Eq. (3) to obtain the relationship in Eq. (9). For isotropic materials, we have

$$Q_{11} = Q_{22} = \frac{E}{1 - \nu^2}$$
  $Q_{12} = \frac{E\nu}{1 - \nu^2}$   $Q_{16} = Q_{26} = 0$   $Q_{66} = \frac{E}{2(1 + \nu)}$ 

For anisotropic materials, the  $Q_{ij}$  formulas are given in a typical textbook on mechanics of composites.

### 4.2 2D Kirchhoff-Love Plate/Shell Model

Kirchhoff originally developed the classical plate model for flat panels based on a set of ad hoc assumptions including the thickness being rigid in the thickness direction, perpendicular to the reference surface, and plane stress assumption. Love later extended the same set of assumptions to curved panels to develop the classical shell model. Since both models are based on same set of assumptions and assume the same model form, we call them collectively as the Kirchhoff-Love model. Here, we use the plate model for illustrative purpose. The kinematics of the Kirchhoff-Love model contains three displacement  $u_1, u_2, u_3$  and six strain variables including the in-plane strains  $\epsilon_{11}, \epsilon_{22}, \epsilon_{12}$  and curvatures  $\kappa_{11}, \kappa_{22}, \kappa_{12}$ . These kinematic variables are all functions of  $x_1$  and  $x_2$ . Specifically for a plate, the strain-displacement relations are given as

$$\epsilon_{11} = \frac{\partial u_1}{\partial x_1} \qquad \epsilon_{22} = \frac{\partial u_2}{\partial x_2} \qquad 2\epsilon_{12} = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}$$

$$\kappa_{11} = -\frac{\partial^2 u_3}{\partial x_1^2} \qquad \kappa_{22} = -\frac{\partial^2 u_3}{\partial x_2^2} \qquad \kappa_{12} = -\frac{\partial^2 u_3}{\partial x_1 \partial x_2}$$

$$(10)$$

The kinetics of the Kirchhoff-Love model contains six stress resultants  $N_{11}$ ,  $N_{22}$ ,  $N_{12}$ ,  $M_{11}$ ,  $M_{22}$ ,  $M_{12}$  with  $N_{11}$ ,  $N_{22}$ ,  $N_{12}$  denoting the in-plane forces and  $M_{11}$ ,  $M_{22}$ ,  $M_{12}$  denoting the moments. These kinetic variables are functions of  $x_1$ ,  $x_2$  and they are governed by the following three equations of equilibrium.

$$\frac{\partial N_{11}}{\partial x_1} + \frac{\partial N_{12}}{\partial x_2} + p_1 = 0$$

$$\frac{\partial N_{21}}{\partial x_1} + \frac{\partial N_{22}}{\partial x_2} + p_2 = 0$$

$$\frac{\partial^2 M_{11}}{\partial x_1^2} + \frac{\partial^2 M_{22}}{\partial x_2^2} + 2\frac{\partial^2 M_{12}}{\partial x_1 \partial x_2} + \frac{\partial q_2}{\partial x_1} - \frac{\partial q_1}{\partial x_2} + p_3 = 0$$
(11)

where  $p_1, p_2, p_3$  are equivalent forces and  $q_1, q_2$  are equivalent moments, distributed over the reference surface.

The constitutive relations of the Kirchhoff-Love model can be expressed using the following six equations.

$$\begin{cases}
N_{11} \\
N_{22} \\
N_{12} \\
M_{11} \\
M_{22} \\
M_{12}
\end{cases} = \begin{bmatrix}
A_{11} & A_{12} & A_{16} & B_{11} & B_{12} & B_{16} \\
A_{12} & A_{22} & A_{26} & B_{12} & B_{22} & B_{26} \\
A_{16} & A_{26} & A_{66} & B_{16} & B_{26} & B_{66} \\
B_{11} & B_{12} & B_{16} & D_{11} & D_{12} & D_{16} \\
B_{12} & B_{22} & B_{26} & D_{12} & D_{22} & D_{26} \\
B_{16} & B_{26} & B_{66} & D_{16} & D_{26} & D_{66}
\end{bmatrix} \begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
2\epsilon_{12} \\
\kappa_{11} \\
\kappa_{22} \\
2\kappa_{12}
\end{pmatrix}$$
(12)

This  $6 \times 6$  matrix is commonly called the plate stiffness matrix and its inverse is called the plate compliance matrix. If a plate is made of a single isotropic material, and the origin of  $x_3$  is chosen to be at the center of the thickness, the constitutive relations can be written as

$$\begin{cases}
N_{11} \\
N_{22} \\
N_{12}
\end{cases} = \frac{Eh}{1 - \nu^2} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1 - \nu}{2} \end{bmatrix} \begin{cases} \epsilon_{11} \\ \epsilon_{22} \\ 2\epsilon_{12} \end{cases} \qquad \begin{cases}
M_{11} \\
M_{22} \\
M_{12} \end{cases} = \frac{Eh^3}{12(1 - \nu^2)} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1 - \nu}{2} \end{bmatrix} \begin{cases} \kappa_{11} \\ \kappa_{22} \\ 2\kappa_{12} \end{cases}$$
(13)

Clearly extension and bending are decoupled for this particular case.

Eqs. (10), (11), and (12) form a system of 15 equations underpinning the Kirchhoff-Love model to be solved along with appropriate boundary conditions for 15 unknowns (3 displacements, six strain variables, and six stress resultants). Kinematics and kinetics remain the same no matter whether the structure is made of metals or composites and these equations have been implemented in many FEA codes which have plate/shell elements. Only difference is that the plate/shell stiffness matrix in Eq. (12) could be fully populated if the plate/shell is made of composites.

It is noted that although the Kirchhoff-Love model was originally developed based on a set of ad hoc assumptions as aforementioned, such assumptions are not used in MSG to derive this model. Also, although we used the familiar terms of A, B, D matrices describing the plate stiffness matrix as those used in the classical lamination theory (CLT), MSG-based Kirchhoff-Love model is not the same as CLT. Thus, the Kirchhoff-Love model here only refers to the model which has 15 field variables of  $x_1, x_2$  governed by the 15 equations in Eqs. (10), (11) and (12). In other words, according to the MSG-based Kirchhoff-Love model, the thickness could be deformed, not necessarily perpendicular to the reference surface, and all six stress components including both in-plane stresses and transverse stresses could exist.

### 4.3 2D Reissner-Mindlin Plate/Shell Model

When the thickness of the panel is not very small with respect to the in-plane dimensions, the Kirchhoff-Love model is inadequate and a refined model is needed. The next refinement is the so-called Reissner-Mindlin model due to independent contribution of Reissner and Mindlin to its development. The kinematics of the Reissner-Mindlin model contains five displacement variables including three displacements  $u_1, u_2, u_3$  and two rotations  $\theta_1, \theta_2$ . This model features eight strain variables including the in-plane strains  $\epsilon_{11}, \epsilon_{22}, \epsilon_{12}$ , curvatures  $\kappa_{11}, \kappa_{22}, \kappa_{12}$ , and transverse shear strains  $\gamma_{12}, \gamma_{13}$ . These kinematic variables are all functions of  $x_1$  and  $x_2$ . Specifically for a plate,

the strain-displacement relations are given as

$$\epsilon_{11} = \frac{\partial u_1}{\partial x_1} \qquad \epsilon_{22} = \frac{\partial u_2}{\partial x_2} \qquad 2\epsilon_{12} = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}$$

$$\kappa_{11} = \frac{\partial \theta_2}{\partial x_1} \qquad \kappa_{22} = -\frac{\partial \theta_1}{\partial x_2} \qquad \kappa_{12} = -\frac{\partial \theta_2}{\partial x_2} - \frac{\partial \theta_1}{\partial x_1}$$

$$\gamma_{13} = \frac{\partial u_3}{\partial x_1} + \theta_2 \qquad \gamma_{23} = \frac{\partial u_3}{\partial x_2} - \theta_1$$

$$(14)$$

The kinetics of the Reissner-Mindlin model contains eight stress resultants  $N_{11}$ ,  $N_{22}$ ,  $N_{12}$ ,  $M_{11}$ ,  $M_{22}$ ,  $M_{12}$ ,  $M_{13}$ ,  $N_{23}$  with  $N_{11}$ ,  $N_{22}$ ,  $N_{12}$  denoting the in-plane forces,  $M_{11}$ ,  $M_{22}$ ,  $M_{12}$  denoting the moments, and  $N_{13}$ ,  $N_{23}$  denoting the transverse shear forces. These kinetic variables are functions of  $x_1$ ,  $x_2$  and they are governed by the following five equations of equilibrium.

$$\frac{\partial N_{11}}{\partial x_1} + \frac{\partial N_{12}}{\partial x_2} + p_1 = 0$$

$$\frac{\partial N_{21}}{\partial x_1} + \frac{\partial N_{22}}{\partial x_2} + p_2 = 0$$

$$\frac{\partial N_{13}}{\partial x_1} + \frac{\partial N_{23}}{\partial x_2} + p_3 = 0$$

$$\frac{\partial M_{12}}{\partial x_1} + \frac{\partial M_{22}}{\partial x_2} - q_1 - N_{23} = 0$$

$$\frac{\partial M_{11}}{\partial x_1} + \frac{\partial M_{21}}{\partial x_2} + q_2 - N_{13} = 0$$
(15)

The constitutive relations of the Reissner-Mindlin model can be expressed using the following eight equations.

$$\begin{cases}
N_{11} \\
N_{22} \\
N_{12} \\
M_{11} \\
M_{22} \\
N_{13} \\
N_{23}
\end{cases} =
\begin{bmatrix}
A_{11} & A_{12} & A_{16} & B_{11} & B_{12} & B_{16} & Y_{11} & Y_{12} \\
A_{12} & A_{22} & A_{26} & B_{12} & B_{22} & B_{26} & Y_{21} & Y_{22} \\
A_{16} & A_{26} & A_{66} & B_{16} & B_{26} & B_{66} & Y_{31} & Y_{32} \\
B_{11} & B_{12} & B_{16} & D_{11} & D_{12} & D_{16} & Y_{41} & Y_{42} \\
B_{12} & B_{22} & B_{26} & D_{12} & D_{22} & D_{26} & Y_{51} & Y_{52} \\
B_{16} & B_{26} & B_{66} & D_{16} & D_{26} & D_{66} & Y_{61} & Y_{62} \\
Y_{11} & Y_{21} & Y_{31} & Y_{41} & Y_{51} & Y_{61} & C_{11} & C_{12} \\
Y_{12} & Y_{22} & Y_{32} & Y_{42} & Y_{52} & Y_{62} & C_{12} & C_{22}
\end{cases}
\end{cases}$$

$$(16)$$

This  $8 \times 8$  matrix is called the plate stiffness matrix and its inverse is called the plate compliance matrix. It is noted that A, B, D matrices could be different from those in Eq. (12) due to possible nonzero  $Y_{ij}$ ,  $i = 1, \ldots, 6$ ; j = 1, 2.

Eqs. (14), (15), and (16) form a system of 21 equations underpinning the Reissner-Mindlin model to be solved along with appropriate boundary conditions for 21 unknowns (5 displacement variables, 8 strain variables, and 8 stress resultants). Kinematics and kinetics remain the same no matter whether the structure is made of metals or composites and these equations have been implemented in many FEA codes which have plate/shell elements. Only difference is that the plate/shell

stiffness matrix in Eq. (16) could be fully populated if the plate/shell is made of composites.

It is noted that although the Reissner-Mindlin model was originally developed based on a set of ad hoc assumptions, such assumptions are not used in MSG to derive this model. Thus, the Reissner-Mindlin model here only refers to the model which has 21 field variables of  $x_1, x_2$  governed by the 21 equations in Eqs. (14), (15) and (16). The deformation and stress state of the structure is not assumed a priori but determined by MSG.

### 4.4 1D Euler-Bernoulli Beam Model

The kinematics of the Euler-Bernoulli beam model contains four displacement variables  $u_1, u_2, u_3, \theta_1$  with  $u_1, u_2, u_3$  describing displacements in three direction and  $\theta_1$  describing the twist angle. This model also features four strain variables including the axial strain  $\gamma_{11}$ , the twist rate  $\kappa_{11}$ , and curvatures  $\kappa_{12}, \kappa_{13}$  around  $x_2$  and  $x_3$ , respectively. These kinematic variables are all functions of  $x_1$  only. The strain-displacement relations are given as

$$\gamma_{11} = \frac{du_1}{dx_1} \qquad \kappa_{11} = \frac{d\theta_1}{dx_1} \qquad \kappa_{12} = -\frac{d^2u_3}{dx_1^2} \qquad \kappa_{13} = \frac{d^2u_2}{dx_1^2}$$
(17)

The kinetics of the Euler-Bernoulli beam model contains four stress resultants  $F_1$ ,  $M_1$ ,  $M_2$ ,  $M_3$  with  $F_1$  denoting the axial force and  $M_1$ ,  $M_2$ ,  $M_3$  denoting the moments about three directions. These kinetic variables are functions of  $x_1$  only and they are governed by the following four equations of equilibrium.

$$\frac{dF_1}{dx_1} + p_1 = 0$$

$$\frac{dM_1}{dx_1} + q_1 = 0$$

$$\frac{d^2M_2}{dx_1^2} + p_3 + \frac{dq_2}{dx_1} = 0$$

$$\frac{d^2M_3}{dx_1^2} - p_2 + \frac{dq_3}{dx_1} = 0$$
(18)

where  $p_1, p_2, p_3$  are equivalent forces and  $q_1, q_2, q_3$  are equivalent moments in three directions, distributed along the reference line.

The constitutive relations of the Euler-Bernoulli beam model can be expressed using the following four equations.

This  $4 \times 4$  matrix is commonly called the beam stiffness matrix and its inverse is called the beam compliance matrix. If a beam is made of a single isotropic material, and the origin of the cross-sectional coordinates  $x_2, x_3$  is chosen to be at the tension center of the cross section and  $x_2, x_3$  align

with the principal bending directions of the beam, the constitutive relations can be written as

$$\begin{cases}
F_1 \\
M_1 \\
M_2 \\
M_3
\end{cases} = \begin{bmatrix}
EA & 0 & 0 & 0 \\
0 & GJ & 0 & 0 \\
0 & 0 & EI_2 & 0 \\
0 & 0 & 0 & EI_3
\end{bmatrix} \begin{cases}
\gamma_{11} \\
\kappa_{11} \\
\kappa_{12} \\
\kappa_{13}
\end{cases}$$
(20)

Clearly the beam stiffness matrix becomes a diagonal matrix for this particular case and the diagonal terms are the well known engineering constants including extension stiffness EA, torsional stiffness GJ, and bending stiffnesses  $EI_2$  and  $EI_3$  for bending about  $x_2$  and  $x_3$  respectively.

Eqs. (17), (18), and (19) form a system of 12 equations underpinning the Euler-Bernoulli model to be solved along with appropriate boundary conditions for 12 unknowns (4 displacement variables, 4 strain variables, and 4 stress resultants). Kinematics and kinetics remain the same no matter whether the structure is made of metals or composites and these equations have been implemented in many FEA codes which have beam elements. In fact, many beam problems, particularly those with a uniform cross section, can be solved analytical using what we have learned in undergraduate mechanics of materials. Only difference is that the beam stiffness matrix in Eq. (19) could be fully populated if the beam is made of composites.

It is noted that although the Euler-Bernoulli model was originally developed based on a set of ad hoc assumptions including the cross section being rigid in plane, perpendicular to the reference line, and uniaxial stress assumption. However, such assumptions are not used in MSG to derive this model. Thus, the Euler-Bernoulli model here only refers to the model which has 12 field variables of  $x_1$  governed by the 12 equations in Eqs. (17), (18) and (19). In other words, according to the MSG-based Euler-Bernoulli model, the cross section could be deformed, not necessarily perpendicular to the reference line, and all six stress components could exist. Actually, the slender structure which is modeled using an MSG-based beam model may not even have clearly defined cross sections. As long as an SG for the slender structure can be defined, an MSG-based beam model can be used for the analysis.

#### 4.5 1D Timoshenko Beam Model

The kinematics of the Timoshenko beam model contains six displacement variables  $u_1, u_2, u_3, \theta_1, \theta_2, \theta_3$  with  $u_1, u_2, u_3$  describing displacements in three directions and  $\theta_1, \theta_2, \theta_3$  describing rotations about three directions. The Timoshenko beam model features six strain variables including the axial strain  $\gamma_{11}$ , transverse shear strains  $\gamma_{12}, \gamma_{13}$ , the twist rate  $\kappa_{11}$ , and curvatures  $\kappa_{12}, \kappa_{13}$ . These kinematic variables are all functions of  $x_1$  only. The strain-displacement relations are given as

$$\gamma_{11} = \frac{du_1}{dx_1} \qquad \gamma_{12} = -\theta_3 + \frac{du_2}{dx_1} \qquad \gamma_{13} = \theta_2 + \frac{du_3}{dx_1} 
\kappa_{11} = \frac{d\theta_1}{dx_1} \qquad \kappa_{12} = \frac{d\theta_2}{dx_1} \qquad \kappa_{13} = \frac{d\theta_3}{dx_1}$$
(21)

The kinetics of the Timoshenko beam model contains six stress resultants  $F_1$ ,  $F_2$ ,  $F_3$ ,  $M_1$ ,  $M_2$ ,  $M_3$  with  $F_1$  denoting the axial force,  $F_2$  and  $F_3$  denoting the transverse shear forces, and  $M_1$ ,  $M_2$ ,  $M_3$ 

denoting the bending moments about three directions. These kinetic variables are functions of  $x_1$  only and they are governed by the following six equations of equilibrium.

$$\frac{dF_1}{dx_1} + p_1 = 0$$

$$\frac{dF_2}{dx_1} + p_2 = 0$$

$$\frac{dF_3}{dx_1} + p_3 = 0$$

$$\frac{dM_1}{dx_1} + q_1 = 0$$

$$\frac{dM_2}{dx_1} - F_3 + q_2 = 0$$

$$\frac{dM_3}{dx_1} + F_2 + q_3 = 0$$
(22)

The constitutive relations of the Timoshenko beam model can be expressed using the following six equations.

$$\begin{cases}
F_1 \\
F_2 \\
F_3 \\
M_1 \\
M_2 \\
M_3
\end{cases} = 
\begin{bmatrix}
C_{11}^b & C_{12}^b & C_{13}^b & C_{14}^b & C_{15}^b & C_{16}^b \\
C_{12}^b & C_{22}^b & C_{23}^b & C_{24}^b & C_{25}^b & C_{26}^b \\
C_{13}^b & C_{23}^b & C_{33}^b & C_{34}^b & C_{35}^b & C_{36}^b \\
C_{14}^b & C_{24}^b & C_{34}^b & C_{44}^b & C_{45}^b & C_{46}^b \\
C_{15}^b & C_{25}^b & C_{35}^b & C_{45}^b & C_{56}^b & C_{56}^b \\
C_{16}^b & C_{26}^b & C_{36}^b & C_{46}^b & C_{56}^b & C_{66}^b
\end{cases} = 
\begin{pmatrix}
\gamma_{11} \\
\gamma_{12} \\
\gamma_{13} \\
\kappa_{11} \\
\kappa_{12} \\
\kappa_{13}
\end{pmatrix} \tag{23}$$

This  $6 \times 6$  matrix is called the beam stiffness matrix and its inverse is called the beam compliance matrix for the Timoshenko model. It is It is noted that  $C_{ij}^b$ , i = 1, 2, 3, 4; j = 1, 2, 3, 4 in this stiffness matrix could be different from those in Eq. (19).

Eqs. (21), (22), and (23) forms a system of 18 equations to be solved along with appropriate boundary conditions for 18 unknowns (6 displacement variables, 6 strain variables, and 6 stress resultants). Kinematics and kinetics remain the same no matter whether the structure is made of metals or composites and these equations have been implemented in many FEA codes which have beam elements. Only difference is that the beam stiffness matrix in Eq. (23) could be fully populated if the beam is made of composites.

It is noted that although the Timoshenko model was originally developed based on a set of ad hoc assumptions including the cross section being rigid in plane, remaining plane during deformation, and uniaxial stress assumption. However, such assumptions are not used in MSG to derive this model. Thus, the Timoshenko model here only refers to the model which has 18 field variables of  $x_1$  governed by the 18 equations in Eqs. (21), (22) and (23).

### 5 Mechanics of Structure Genome (MSG)

### 5.1 The Concept of Structure Genome

Inspired by the fundamental role of a genome for an organism's growth and development, we extrapolate this word into non-biological contexts to define SG as the *smallest mathematical building block* of a structure. SG contains all the constitutive information needed for a structure in the same fashion as the genome contains all the genetic information for an organism. It is noted that if one is using SwiftComp<sup>TM</sup> for multiphysics behavior other than structural behavior, an SG should be interpreted as a fundamental building block (or genome) of the material instead.

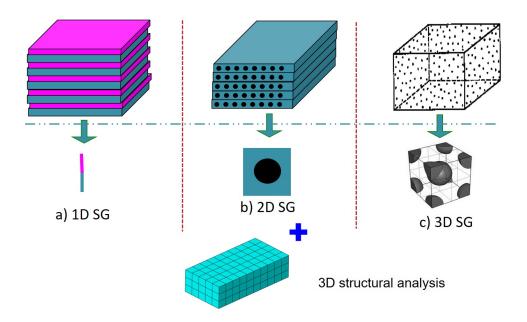


Figure 3: Analysis of 3D heterogeneous structures approximated by a constitutive modeling over SG and a corresponding 3D macroscopic structural analysis.

### 5.2 SG for 3D Structures

As shown in Figure 3, analyses of 3D heterogeneous structures can be approximated by a 3D macroscopic structural analysis with the material properties provided by a constitutive modeling of an SG. For 3D structures, SG serves a similar role as the representative volume element (RVE) in micromechanics. However, they are significantly different so that the new term, SG, is used to avoid confusion. For example, for a structure made of composites featuring 1D heterogeneity (e.g. binary composites made of two alternating layers, Figure 3a), the SG will be a straight line with two segments denoting corresponding phases. One can mathematically repeat this line in-plane to build the two layers of the binary composite, and then repeat the binary composite out of plane to build the entire structure. Another possible application is to model a laminate as an equivalent

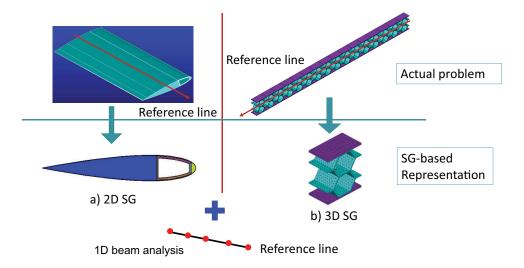


Figure 4: Analysis of beam-like structures approximated by a constitutive modeling over SG and a corresponding 1D beam analysis.

anisotropic homogeneous solid. The transverse normal line is the 1D SG for the laminate. The constitutive modeling over the 1D SG can 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 3b), the SG will be 2D. Although 2D RVEs are also used in micromechanics, only in-plane properties and in-plane local fields can be obtained from common RVE-based models. If the complete set of properties are needed for the 3D structural analysis, a 3D RVE is usually required [6], while a 2D domain is sufficient if it is modeled using SG-based models (Figure 3b). For a structure made of composites featuring 3D heterogeneity (e.g. particle reinforced composites, Figure 3c), the SG will be a 3D volume. Although a 3D SG for 3D structures represents the most similar case to RVE, boundary conditions in terms of displacements and tractions indispensable in RVE-based models are not needed for SG-based models.

### 5.3 SG for Dimensionally Reducible Structures

SG also allows direct connection of microstructure with the beam/plate/shell analyses. For example, the structural analysis of slender (beam-like) structures can use beam elements (Figure 4). If the beam has uniform cross sections which could be made of isotropic homogeneous materials or anisotropic heterogeneous materials (Figure 4a), its SG is the 2D cross-sectional domain because the cross section can be projected along the beam reference line to form the beam-like structure. This inspires a new perspective toward beam modeling, a traditional branch of structural mechanics. If the beam reference line is considered as a 1D continuum, every material point of this continuum has a cross section as its microstructure. In other words, constitutive modeling for beams can be effectively viewed as an application of micromechanics. If the beam is also heterogeneous in the spanwise direction (Figure 4b), a 3D SG is needed to describe the microstructure of the 1D con-

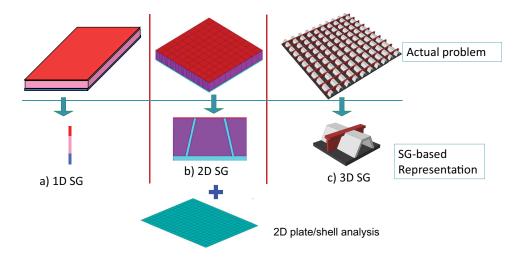


Figure 5: Analysis of plate-like structures approximated by a constitutive modeling over SG and a corresponding 2D plate analysis.

tinuum, the behavior of which is governed by the 1D beam analysis. The constitutive modeling over an SG should compute the beam stiffness for the beam analysis, and also the complete 3D displacement, stress, and strain fields within the original structure. The concept of SG provides a unified treatment of structural modeling and micromechanics modeling and enables us to collapse the cross section or a 3D beam segment into a material point for a beam analysis over the reference line with a possible, fully populated stiffness matrix simultaneously accounting for all the deformation modes of a certain model such as the Euler-Bernoulli beam model (extension, torsion, and bending in two directions) or the Timoshenko beam model (extension, torsion, bending in two directions, and shear in two directions). The beam theory constructed this way can easily handle buildup structures as long as their external contours look like a beam such as high aspect ratio wings, or as long as the analyst wants to model a structure using a beam element.

If the structural analysis uses plate/shell elements, SG can also be chosen properly. For illustrative purpose, typical SGs of plate-like structures are sketched in Figure 5. If the plate-like structures feature no in-plane heterogeneities (in other words, the structure is assumed to be made of homogeneous layers) (Figure 5a), the SG is the transverse normal line with each segment denoting the corresponding layer. For a sandwich panel with a core corrugated in one direction (Figure 5b), the SG is 2D. If the panel is heterogeneous in both in-plane directions (Figure 5c), such as a stiffened panel with stiffeners running in both directions, the SG is 3D. Despite the different dimensionalities of the SGs, the constitutive modeling should output structural properties for the corresponding structural analysis (such as the A, B, and D matrices for the Kirchhoff-Love plate model) and relations to express the original 3D fields in terms of the global behavior (e.g. moments, curvatures, etc.) obtained from the plate/shell analysis. It is known that theories of plates/shells traditionally belong to structural mechanics, but the constitutive modeling of these structures can be treated as special micromechanics applications using the SG concept. For a plate/shell-like structure, if the reference surface is considered as a 2D continuum, every material point of this continuum has

an associated SG as its microstructure. Plate/shell models constructed using the SG concept can handle buildup structures as long as their external contours look like plates or shells or we want to model a piece of structure using plate or shell elements.

It is easy to identify SGs for periodic structures as shown in Figures. 3, 4, and 5. For structures which are not globally periodic, we usually 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. 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, the SG should be interpreted as the smallest mathematical building block necessary to represent the nonlinear behavior.

SG serves as the link between the original structure with microscopic details and the macroscopic structural analysis. Here, the terms "microstructure" and "microscopic details" are used in a general sense: any details explicitly existing in an SG but not in the macroscopic structural analysis are termed microscopic details. The real structure with microscopic details is termed as the original structure and the structure used in the macroscopic structural analysis is termed as the macroscopic structural model. It is also interesting to point out the relation between the SG concept and the idea of sub-structuring or super-element, which is commonly used in engineering. A line element in the global analysis could correspond to a box beam made of four laminated walls, and a surface element could correspond to a sandwich panel with laminated face sheets and a corrugated core. For these cases, MSG provides a rigorous and systematic approach to compute the constitutive models for the line and surface elements and the local fields within the original structures.

### 5.4 MSG-based Multiscale Structural Modeling

The multiscale structural modeling approach based on MSG can be used to fill the gap between materials genome and macroscopic structural analysis and can directly connect with simple structural elements (beams/plates/shells/3D solid elements) available in standard FEA software packages (see Figure 2).

As shown in Figure 6, MSG starts from the original model, say formulated in terms of 3D continuum mechanics. We first identify SG as the basic building block of the structure, then use the principle of minimum information loss (PMIL) to decouple the original problem to a constitutive modeling over the SG and a structural analysis. The constitutive modeling has been implemented in SwiftComp<sup>TM</sup>. SwiftComp<sup>TM</sup> will provide the constitutive models needed in the structural analysis to obtain the global structural behavior and also dehomogenization relations to obtain the local fields within the original structure. The structural analysis can be formulated as a geometrically exact continuum theory and all the approximations are confined in the constitutive modeling, accuracy of which is guaranteed to be the best by PMIL. This theory not only performs homogenization to obtain the constitutive models needed for the structural analysis, but performs dehomogenization to compute pointwise displacements/stresses/strains within the original structure which are critical for strength and failure predictions.

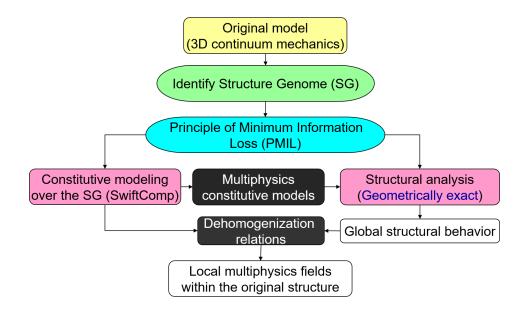


Figure 6: Work flow of MSG-based multiscale modeling.

As the macroscopic structural analysis can be easily handled by standard FEA software packages, this SwiftComp<sup>TM</sup>-empowered multiscale structural modeling approach enables these FEA software packages to model composites as a *black aluminum* in the macroscopic structural analysis with minimized loss of accuracy. But this "black aluminum" is an anisotropic homogeneous continuum, not an isotropic material as traditionally implied by this popular term. The unique features of this multiscale modeling approach based on SwiftComp<sup>TM</sup> are:

- Use SG to fill the gap between materials genome and the macroscopic structural analysis. Intellectually, SG enables us to view constitutive modeling of structures as an application of micromechanics. Technically, SG empowers us to systematically model complex buildup structures with heterogeneities of length scales comparable to the smallest structural dimension.
- Use PMIL based on the powerful variational asymptotic method (VAM) to avoid apriori assumptions commonly invoked in other approaches, providing the most mathematical rigor and the best engineering generality.
- Decouple the original problem into two sets of analyses: a constitutive modeling and a structural analysis. This allows the structural analysis to be formulated exactly as a general (1D, 2D, or 3D) continuum, the analysis of which is readily available in commercial FEA software packages and confines all approximations to the constitutive modeling, the accuracy of which is guaranteed to be the best by PMIL.
- Maintain the engineering simplicity and legacy by repacking the refined asymptotically correct functionals into common engineering models so that models constructed using this approach can be incorporated into standard FEA software packages.



Figure 7: 1D element nodal numbering

Since most of the theoretical details of SG are presented in its relevant publications [1, 7, 2, 3], this manual will only serve to help readers get started using SwiftComp<sup>TM</sup> to solve their own constitutive modeling problems. In the following, we will address its conventions, inputs, outputs, maintenance, and tech support.

## 6 SwiftComp $^{TM}$ Conventions

To understand the inputs and interpret outputs of the program correctly, we need to explain some conventions used in the SwiftComp<sup>TM</sup> code.

### 6.1 Elements

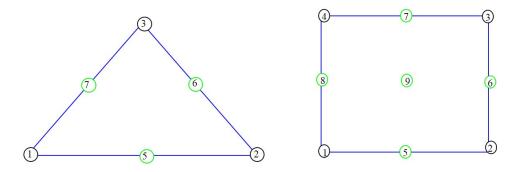


Figure 8: 2D element nodal numbering

SwiftComp<sup>TM</sup> can use two-noded, three-noded, four-noded, or five-noded elements for 1D SGs as shown in Figure 7. Nodes 3, 4, 5 are optional and one or more of these nodes can be missing for a valid 1D element. It is recommended to use 2-noded elements for 3D structures with a 1D SG (see Figure 3a) and 5-noded elements for 2D plate/shell models with a 1D SG (see Figure 5a).

2D SGs can be meshed using either triangular elements or quadrilateral elements as shown in Figure 8. It is also shown in the figure that SwiftComp<sup>TM</sup> numbers the nodes of each 2D elements in the counterclockwise direction. Nodes 1, 2, and 3 of the triangular elements and nodes 1, 2, 3, and 4 of the quadrilateral elements are at the corners. For triangular element, the fourth node is zero to inform SwiftComp<sup>TM</sup> that it is a triangular element. Nodes 5, 6, 7 of the triangular elements and nodes 5, 6, 7, 8, 9 of quadrilateral elements are optional. Any one or more of these nodes can be missing for a valid 2D element.

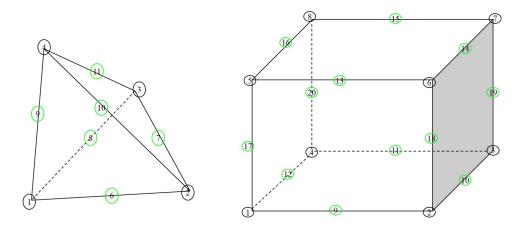


Figure 9: 3D element nodal numbering

SwiftComp<sup>TM</sup> meshes 3D SGs using either tetrahedral elements or brick elements as shown in Figure 9. Note at least the corner nodes should exist and for tetrahedral elements, the fifth node is zero to inform SwiftComp<sup>TM</sup> that it is a tetrahedral element. The nodes other than the corners are optional. Any one or more of these nodes can be missing for a valid 3D element.

# 6.2 Local Coordinate System, Elemental Coordinate System, and Material Coordinate System

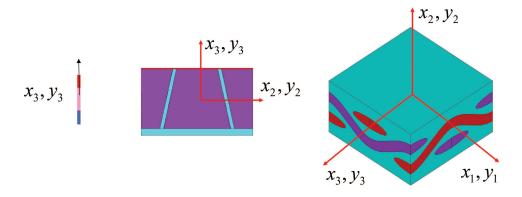


Figure 10: Local coordinate system describing SG

First, SwiftComp<sup>TM</sup> uses a right-hand Cartesian coordinate system, also called the *local coordinate system*, denoted as  $y_1, y_2$  and  $y_3$ , to describe a 3D SG,  $y_2$  and  $y_3$  to describe a 2D SG, and  $y_3$  to describe a 1D SG (see Figure 10).  $y_1, y_2, y_3$  are parallel to the *global coordinates*  $x_1, x_2, x_3$ , respectively. The global coordinates  $x_1, x_2, x_3$  are used to describe the original structure and the macroscopic structure. Note that if the material properties are provided in a coordinate system different from  $y_1, y_2, y_3$ , an additional coordinate system called the *material coordinate system* should be defined and a transformation of the material properties from the material coordinate systems

into those expressed in the local coordinate system is automatically carried out by SwiftComp<sup>TM</sup>.

In SwiftComp<sup>TM</sup>, an elemental coordinate system  $y_i'$  can be defined for each element denoted by three points a, b, c, with the line from point c to point a denoting  $y_1'$  direction and the line from point c to point b in the  $y_1' - y_2'$  plane; see Figure 11 for a sketch. Speaking in the language of vectors, the new coordinate system is defined by three points with position vectors in  $y_i$  coordinate system by a, b, c. a - c denotes  $\hat{e}_1'$ , b - c is a vector in the  $y_1' - y_2'$  plane. With this information, one can compute the direction cosine matrix relating  $y_i$  to  $y_i'$  according to the following steps:

- Obtain  $\hat{e}'_1$  through normalization of a c:  $\hat{e}'_1 = \frac{a c}{|a c|}$ ;
- Obtain  $\hat{e}_3'$  through normalization of the cross product of  $\hat{e}_1'$  and b-c:  $\hat{e}_3' = \frac{\hat{e}_1' \times (b-c)}{|\hat{e}_1' \times (b-c)|}$ ;
- Obtain  $\hat{e}'_2$  through the cross product of  $\hat{e}'_3$  and  $\hat{e}'_1$ :  $\hat{e}'_2 = \hat{e}'_3 \times \hat{e}'_1$ .

SwiftComp<sup>TM</sup> allows the user to define the material properties in the local coordinate system  $y_i$  or in the material coordinate system. The material coordinate system could be the elemental coordinate system or a coordinate system defined in such a way that it can be obtained by a simple rotation about  $y'_3$  of the elemental coordinate system. Clearly for composite laminates, this simple rotation corresponds to the layup angle.

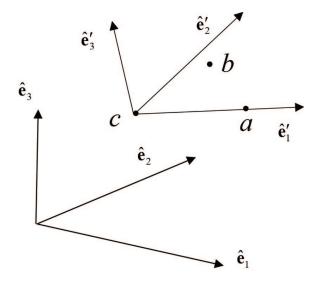


Figure 11: Elemental coordinate system defined by three points.

#### 6.3 Constituent Constitutive Models

Generally speaking, the constituents contained in a SG could be responsive to thermal, mechanical, electric, and magnetic fields. If these effects are not coupled, the linear elastic behavior can be modeled using the generalized Hooke's law in Eq. (3).

To deal with uncoupled thermal, electric, and magnetic effects, conduction can be modeled using the following constitutive relation:

where  $q_i$  is the heat flux,  $k_{ij}$  is the conductivity, and  $T_{,i}$  is the gradient of the temperature T. Since conduction is mathematically analogous to electrostatics, magnetostatics, and diffusion, SwiftComp<sup>TM</sup> can also be used to predict effective dielectric, magnetic, and diffusive properties of composite materials and the corresponding local fields. For example, to obtain the effective dielectric properties, we just need to let  $q_i$  denote the electric displacements, T denote the electric potential, and  $k_{ij}$  denote the corresponding dielectric properties.

For coupled mutliphysics modeling, we will have piezoelectric and piezomagnetic effects as well as pyroelectric, pyromagnetic, and electromagnetic effects. For linear behavior among all these fields, the constitutive equations can be expressed as:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} - e_{kij}E_k - q_{kij}H_k + \Lambda_{ij}\theta$$

$$D_i = e_{ikl}\varepsilon_{kl} + k_{ik}E_k + a_{ik}H_k + p_i\theta$$

$$B_i = q_{ikl}\varepsilon_{kl} + a_{ik}E_k + \mu_{ik}H_k + m_i\theta$$
(25)

where  $C_{ijkl}$ ,  $e_{kij}$ ,  $q_{kij}$ , and  $\Lambda_{ij}$  are the elastic, the piezoelectric, the piezomagnetic, and the thermal stress tensors, respectively (note that  $\Lambda_{ij} = -C_{ijkl}\alpha_{kl}$  with  $\alpha_{kl}$  as the thermal expansion tensor);  $\sigma_{ij}$  and  $\varepsilon_{ij}$  are the stress tensor and strain tensor, respectively;  $k_{ik}$ ,  $a_{ik}$ , and  $\mu_{ik}$  are the dielectric, electromagnetic, and magnetic permeability tensors, respectively; and  $p_i$  and  $m_i$  are the pyroelectric and pyromagnetic vectors, and  $D_i$ ,  $E_k$ ,  $B_i$ , and  $H_k$  are the electric displacement, electric field, magnetic induction, and magnetic field vectors, respectively.  $\theta$  denotes the difference between the actual temperature and the reference temperature. SwiftComp<sup>TM</sup> does not restrict  $\theta$  to be small. If  $\theta$  is not small,  $\Lambda_{ij}$ ,  $p_i$ ,  $m_i$  are not the tangent or instantaneous properties, but the secant properties which are defined as average over a change of temperature. For example, let  $\alpha_t(T)$  denote the tangent or instantaneous coefficient of thermal expansion (CTE), the secant CTE is defined as

$$\alpha(T) = \frac{1}{T - T_1} \int_{T_1}^{T} \alpha_t(\zeta) d\zeta = \frac{1}{\theta} \int_{T_1}^{T_1 + \theta} \alpha_t(\zeta) d\zeta \tag{26}$$

with  $T_1$  as the reference temperature and  $\theta = T - T_1$ . For convenience, SwiftComp<sup>TM</sup> uses tangent or instantaneous properties for  $\alpha_{ij}, p_i, m_i$  as inputs and computes the secant properties internally for constitutive modeling of temperature dependent properties.

Linear multiphysics behavior is modeled based on the following energy functional corresponding to the constitutive equation in Eq. (25):

$$U = \frac{1}{2} \epsilon^T L \epsilon + \epsilon^T \beta \theta - \int_{T_1}^T \int_{T_1}^{\zeta} \frac{c_{\epsilon}(0, \rho)}{\rho} d\rho d\zeta$$
 (27)

where

$$\epsilon = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{22} & \varepsilon_{33} & 2\varepsilon_{23} & 2\varepsilon_{13} & 2\varepsilon_{12} & -E_1 & -E_2 & -E_3 & -H_1 & -H_2 & -H_3 \end{bmatrix}^T \tag{28}$$

is a multiphysical field vector containing the 3D strain field  $\varepsilon_{ij}$ , the 3D electric field  $E_i$ , and the 3D magnetic field  $H_i$ . The conjugate multiphysical field vector  $\sigma$  can be expressed as

$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{33} & \sigma_{23} & \sigma_{13} & \sigma_{12} & D_1 & D_2 & D_3 & B_1 & B_2 & B_3 \end{bmatrix}^T$$
 (29)

L is a  $12 \times 12$  multiphysics matrix containing all the necessary material constants for characterizing fully coupled thermoelectromagnetoelastic materials such that

$$L = \begin{bmatrix} C & e & q \\ e^T & -k & -a \\ q^T & -a^T & -\mu \end{bmatrix}$$

$$(30)$$

where C is a  $6 \times 6$  submatrix for elastic constants, e is a  $6 \times 3$  submatrix for piezoelectric coefficients, q is a  $6 \times 3$  submatrix for piezomagnetic coefficients, k is a  $3 \times 3$  submatrix for dielectric coefficients, k is a k is a k 3 submatrix for magnetic permeability. Note k is a k 3 submatrix for magnetic permeability. Note k is a k 3 submatrix for magnetic permeability. Note k is a k 3 submatrix for magnetic form of the k 12 matrix is as follows

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} & e_{11} & e_{21} & e_{31} & q_{11} & q_{21} & q_{31} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} & e_{12} & e_{22} & e_{32} & q_{12} & q_{22} & q_{32} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} & e_{13} & e_{23} & e_{33} & q_{13} & q_{23} & q_{33} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} & e_{14} & e_{24} & e_{34} & q_{14} & q_{24} & q_{34} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} & e_{15} & e_{25} & e_{35} & q_{15} & q_{25} & q_{35} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} & e_{16} & e_{26} & e_{36} & q_{16} & q_{26} & q_{36} \\ e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} & -k_{11} & -k_{12} & -k_{13} & -a_{11} & -a_{12} & -a_{13} \\ e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} & -k_{12} & -k_{22} & -k_{23} & -a_{12} & -a_{22} & -a_{23} \\ e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} & -k_{13} & -k_{23} & -k_{33} & -a_{13} & -a_{23} & -a_{33} \\ q_{11} & q_{12} & q_{13} & q_{14} & q_{15} & q_{16} & -a_{11} & -a_{21} & -a_{31} & -\mu_{11} & -\mu_{12} & -\mu_{13} \\ q_{21} & q_{22} & q_{23} & q_{24} & q_{25} & q_{26} & -a_{12} & -a_{22} & -a_{32} & -\mu_{12} & -\mu_{22} & -\mu_{23} \\ q_{31} & q_{32} & q_{33} & q_{34} & q_{35} & q_{36} & -a_{13} & -a_{23} & -a_{33} & -\mu_{13} & -\mu_{23} & -\mu_{33} \end{bmatrix}$$

Other terms in Eq. (27) include  $\beta$ , which is a  $12 \times 1$  matrix containing the second-order thermal stress tensor  $\Lambda_{ij}$ , the vector of pyroelectric  $p_i$ , and the vector of pyromagnetic  $m_i$  expressed as

$$\beta = \begin{bmatrix} \Lambda_{11} & \Lambda_{22} & \Lambda_{33} & \Lambda_{23} & \Lambda_{13} & \Lambda_{12} & p_1 & p_2 & p_3 & m_1 & m_2 & m_3 \end{bmatrix}^T$$
(32)

The coefficient in the last term  $c_{\epsilon}$  is the specific heat per unit volume at constant strain. Note in the input, we actually input the coefficients of thermal expansion  $\alpha_{kl}$  to be consistent with thermoelastic analysis. The code automatically computes  $\Lambda_{ij}$  according to the following formula:

$$\begin{cases}
\Lambda_{11} \\
\Lambda_{22} \\
\Lambda_{33} \\
\Lambda_{23} \\
\Lambda_{13} \\
\Lambda_{12}
\end{cases} = -
\begin{bmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\
C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\
C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\
C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66}
\end{bmatrix}
\begin{pmatrix}
\alpha_{11} \\
\alpha_{22} \\
\alpha_{33} \\
2\alpha_{23} \\
2\alpha_{13} \\
2\alpha_{12}
\end{pmatrix}$$
(33)

Note in the right hand side, the off diagonal CTEs are multiplied by 2 so that we have  $2\alpha_{12}$ ,  $2\alpha_{13}$ ,  $2\alpha_{23}$  according to the engineering notation.

As it is a constant confusion among users regarding the units used in the multiphysics modeling, we will provide a detailed description of those units. According to the International Standard unit system, we use  $\mathbf{Pa}$  (i.e.,  $\mathbf{N/m^2}$ ) for the elastic constants  $C_{ijkl}$  and the stress field  $\sigma_{ij}$  (note the strain field  $\varepsilon_{ij}$  is unitless),  $\mathbf{C/m^2}$  for piezoelectric constants  $e_{ijk}$  and electric displacement  $D_i$ ,  $\mathbf{N/(A \cdot m)}$  for piezomagnetic constants  $q_{ijk}$  and magnetic induction  $B_i$ ,  $\mathbf{C/(V \cdot m)}$  for dielectric constants  $k_{ij}$ ,  $\mathbf{N/A^2}$  (or  $\mathbf{N \cdot s^2/C^2}$ ) for magnetic permeability  $\mu_{ij}$ ,  $\mathbf{C/(A \cdot m)}$  for electromagnetic coefficients  $a_{ij}$ ,  $\mathbf{V/m}$  for electric field  $E_i$ ,  $\mathbf{A/m}$  for magnetic field  $H_i$ ,  $\mathbf{K}$  for the temperature field  $\theta$  (note °C has the same unit dimension as  $\mathbf{K}$ ),  $\mathbf{1/K}$  for thermal expansion coefficients  $\alpha_{ij}$  (correspondingly  $\mathbf{Pa/K}$  for thermal stress coefficients  $\Lambda_{ij}$ ),  $\mathbf{C/m^2 \cdot K}$  for pyroelectric constants  $p_i$ ,  $\mathbf{N/(A \cdot m \cdot K)}$  for pyromagnetic  $m_i$ , and  $\mathbf{J/(m^3 \cdot K)}$  for the specific heat  $c_{\epsilon}$ . With all these units, the energy density U will be in the unit of  $\mathbf{N/m^2}$ , which is the same as  $\mathbf{J/m^3}$ . Note  $\mathbf{N=C \cdot V/m}$  and  $\mathbf{J=N \cdot m}$ .

Although the units aforementioned are consistent with each other, direct use of these units will introduce an extremely ill-conditioned material matrix L as for regular materials, we have  $C_{ijkl}$  in the order of  $10^{11}$ , while  $k_{ij}$  in the order of  $10^{-9}$ . Proper scaling is needed even if double precision is used in computing. To this end, we define  $E_i^* = \frac{E_i}{10^9}$ ,  $H_i^* = \frac{H_i}{10^9}$ , then the energy density in Eq. (27) can be rewritten as:

$$\frac{U}{10^9} = \frac{1}{2} \left\{ \begin{array}{ccc} \varepsilon \\ -E^* \\ -H^* \end{array} \right\}^T \left[ \begin{array}{ccc} C^* & e & q \\ e^T & -k^* & -a^* \\ q^T & -a^{*T} & -\mu^* \end{array} \right] \left\{ \begin{array}{c} \varepsilon \\ -E^* \\ -H^* \end{array} \right\} + \left\{ \begin{array}{c} \varepsilon \\ -E^* \\ -H^* \end{array} \right\}^T \left\{ \begin{array}{c} -C^*\alpha \\ p \\ m \end{array} \right\} \theta - \int_{T_1}^T \int_{T_1}^{\zeta} \frac{c_{\epsilon}^*(0,\rho)}{\rho} d\rho d\zeta \tag{34}$$

with

$$C^* = \frac{C}{10^9}$$
  $c_{\epsilon}^* = \frac{c_{\epsilon}}{10^9}$   $k^* = k \times 10^9$   $a^* = a \times 10^9$   $\mu^* = \mu \times 10^9$  (35)

The generalized Hooke's law given in Eq. (25) can be rewritten in the following matrix form:

$$\sigma^* = C^* \varepsilon - eE^* - qH^* + \Lambda^* \theta$$

$$D = e^T \varepsilon + k^* E^* + a^* H^* + p_i \theta$$

$$B = q^T \varepsilon + a^{*T} E^* + \mu^* H^* + m_i \theta$$
(36)

# 7 SwiftComp<sup>TM</sup> Execution

SwiftComp<sup>TM</sup> along with a simple graphic user interface (GUI) based on  $Gmsh^8$  is available on cdmHUB (https://cdmhub.org/resources/scstandard). To model with Textile composites, SwiftComp<sup>TM</sup> is integrated with TexGen<sup>9</sup> which is also available on cdmHUB (https://cdmhub.org/resources/texgen4sc). One only needs a browser connected to the Internet to execute the codes. One can also request a copy of SwiftComp<sup>TM</sup> installed on their own computer.

SwiftComp<sup>TM</sup> is distributed in the form of SwiftCompx.xReleasePCMM-DD-YEAR.exe for Windows operating systems with "x.x" denotes the version number. Double click the exe file and follow the setup wizard is all you need to do for installation. More details can refer to the Readme file. The Linux version of SwiftComp<sup>TM</sup> is distributed in the form of SwiftCompx.xReleaseLinuxMM-DD-YEAR.zip. Unzip the file SwiftCompx.xReleaseLinuxMM-DD-YEAR.zip into a folder of your choice is all you need to do for installing SwiftComp<sup>TM</sup>More details can refer to the Readme file.

Currently, we only provide executables for computers with Windows or Linux OS. The Gmsh-based GUI, TexGen-bsed GUI, and interfaces with other commercial FEA software packages such as ANSYS, ABAQUS, NASTRAN can also be freely downloaded from cdmHUB.org. ANSYS-SwiftComp GUI can be found at https://cdmhub.org/resources/1136. ABAQUS-SwiftComp GUI can be found at https://cdmhub.org/resources/1134.

Without a graphic user interface, SwiftComp<sup>TM</sup> should be executed under command line. For example in Windows systems, using the system command cmd to bring up the command line window. Then use the system command cd to enter the right folder where the input files are in. Then type SwiftComp arg1 arg2 arg3 arg4, where SwiftComp is the command name of SwiftComp<sup>TM</sup>. arg1 is the complete input file name (including the extension), arg2 denotes the macroscopic model to be constructed (1D for a beam model, 2D for a plate/shell model, and 3D for a 3D model). arg3 denotes whether homogenization, dehomogenization, or failure analysis will be carried out with H for homogenization, L for dehomogenization, LG for dehomogenization with local results written in Gmsh format, F for initial failure strength analysis, FE for initial failure envelope, FI for initial failure indexes and strength ratios, HA for homogenization of aperiodic structures, LA for dehomogenization of aperiodic structures, and LAG for dehomogenization of aperiodic structures with local results written in Gmsh format. arq4 denotes whether to use reduced integration for certain elements: R for reduced integration, no arguments for full integration. For example, one wants to construct a 3D model using the input file test.sc, then the command SwiftComp test.sc 3D H should be used for homogenization run. If local fields are also desired, the command SwiftComp test.sc 3D L should be used for the dehomogenization run. Note for a specific input file, dehomogenization and initial failure related analyses (arg3=F, FE, or FI) can only be carried out after at least one homogenization run and a corresponding file with extension \*.glb storing extra inputs needed for dehomogenization and initial failure related analyses should also exist in the same folder. For example for the input file test.sc, we should have also prepared a file named test.sc, qlb with details described later for a successful dehomogenization or initial failure related analyses run.

 $SwiftComp^{TM}$  inputs are in free format which means that the entries in input files can be

separated by comma, space, and/or tab, scientific notation such as 1.0E-5 can be used. Since SwiftComp<sup>TM</sup> calculation is carried out using double precision, it can also handle inputs up to 15 significant digits.

### 8 SwiftComp<sup>TM</sup> Inputs for Homogenization Run

Although general-purpose preprocessors can been developed to prepare SwiftComp<sup>TM</sup> input files, it is still beneficial for advanced users, particularly those who want to embed SwiftComp<sup>TM</sup> in their own software environments, to understand the meaning of the input data.

### 8.1 Extra Inputs for Dimensionally Reducible Structures

To construct a beam/plate/shell model, the beginning of the input file has two extra lines for a plate/shell model, and three extra lines for a beam model. The first line of the input file is an integer to denote a specific model. If it is 0, it will construct a classical model (Euler-Bernoulli beam model or Kirchhoff-Love plate/shell model). If it is 1, it will construct a shear refined model (Timoshenko beam model or Reissner-Mindlin plate/shell model). For a beam model, it can also be 2, indicating a Vlasov beam model, or 3 indicating a beam model with the trapeze effect.

The next line has three real numbers  $(k_{11}, k_{12}, k_{13} \text{ for beams})$  or two real numbers  $(k_{12}, k_{21} \text{ for shells})$  as the initial twist/curvatures of the structure. If the structure is initially straight, zeroes should be provided instead.

To construct a beam model, two real numbers will be additionally provided on the third line as the parameters to specify an SG which is an oblique cross section, see Figure 12 for a sketch of such a cross section. The first number is cosine of the angle between normal of the oblique section  $(y_1)$  and beam axis  $x_1$ . The second number is cosine of the angle between  $y_2$  of the oblique section and beam axis  $(x_1)$ . The summation of the square of these two numbers should not be greater than 1.0 in double precision. The inputs including coordinates, material properties, etc. and the outputs including mass matrix, stiffness matrix, etc. are given in the oblique system, the  $y_i$  coordinate system as shown in Figure 12. For normal cross sections, we provide 1.0 0.0 on this line instead.

### 8.2 Inputs for All Structural Models

The following line (note: to construct a 3D structural model, the previous three lines do not exist and the input file starts from this line.) has four integers providing the problem control parameters as:

analysis elem\_flag trans\_flag temp\_flag

The parameter *analysis* is an integer denoting the type of analysis: 0-elastic; 1-thermoelastic; 2-conduction; 3-piezoeletric/piezomagnetic; 4-thermopiezoeletric/thermopiezomagnetic; 5-piezoeletromagnetic; 6-thermopiezoeletromagnetic. It is pointed out here that piezoelectric effects are mathematically equivalent to piezomagnetic effects. In other words, the same equation or code used for

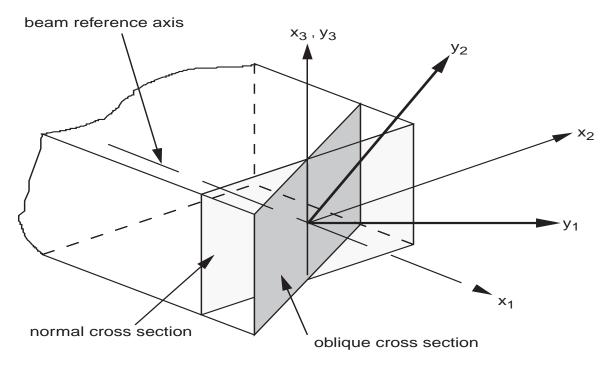


Figure 12: Sketch of an oblique reference cross section

modeling piezoelectric materials can be used to model piezomagnetic materials if we replace electric displacement  $D_i$  with magnetic induction  $B_i$ , electric field  $E_i$  with magnetic field  $H_i$ , piezoelectric properties  $e_{kij}$  with piezomagnetic properties  $q_{kij}$ , pyroelectric properties  $p_i$  with pyromagnetic properties  $p_i$ . Later, for analysis=3 or 4, in the inputs we used piezoelectric materials as example. It is directly applicable to piezomagnetic materials.

The parameter *elem\_flag* is an integer denoting the type of elements. If *elem\_flag* is equal to 0, the regular elements as shown in Figures 7, 8, 9 will be used for 1D, 2D or 3D SGs. If it is equal to 1, elements with one dimension degenerated will be used to model the SG. For example, 2D shell elements based on relative degrees of freedom will be used to mesh a 3D SG or 1D elements will be used to mesh a 2D SG. If it is equal to 2, 1D elements will be used to mesh a 3D SG. For example, 1D beam elements can be used to model a 3D SG composed of slender truss-like members. Currently only regular elements are implemented.

The parameter trans\_flag is an integer denoting whether transformation of the element orientation is needed. If trans\_flag is equal to 0, element orientation is the same as the problem coordinate system and transformation is not needed. If it is equal to 1, elemental coordinate systems are defined for each element and elemental orientations will be provided in a later block for the transformation.

The parameter  $temp\_flag$  is an integer denoting whether the temperature is uniform within the SG. For thermally coupled analysis (analysis=1, 4, 6), if  $temp\_flag$  is equal to 0, temperature

distribution within SG is uniform; if it is equal to 1, temperature distribution is not uniform and nodal temperature should be provided to describe the temperature field. Note this input is used only if it is a thermally coupled analysis.

If the SG is aperiodic or partially periodic, the next line will list three integers arranged as:  $py1 \ py2 \ py3$ 

where py1, py2 py3 could be 1, or 0 indicating whether it is aperiodic or periodic along  $y_1, y_2, y_3$  directions, respectively. For example, for a 3D SG which is aperiodic along  $y_2$  direction, we will have

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It noted that for the 2D plate/shell model, only  $y_1$  or  $y_2$  can be periodic or aperiodic and for the 1D beam model, only  $y_1$  can be periodic or aperiodic.

The next line lists six integers arranged as:

nSG nnode nelem nmate nslave nlayer

where nSG is the dimensionality of the SG, nnode is the total number of nodes, nelem is the total number of elements, nmate is the total number of material types, nslave is the number of slave nodes on periodic boundaries for periodic microstructures, and nlayer is the total number of layers defined by different types of materials and layup angle. If nslave=0, SwiftComp<sup>TM</sup> will search for corresponding node on periodic boundaries. For this reason, the SG must be regular rectangles (for 2D SG) or cuboids (for 3D SG) with the FE mesh having corresponding nodes on periodic edges. For other periodic SG shapes, the paired nodes on corresponding boundaries must be provided through setting nslave not equal to zero.

The next nnode lines are the coordinates for each node arranged as:  $node\_no\ y_1\ y_2\ y_3$ 

where  $node\_no$  is an integer representing the unique number assigned to each node and  $y_1$ ,  $y_2$ ,  $y_3$  are three real numbers describing the location  $(y_1, y_2, y_3)$  of the node (only  $y_3$  exists for 1D SGs, and  $y_2$  and  $y_3$  exist for 2D SGs). Arrangement of  $node\_no$  is not necessary to be consecutive, but all nodes from 1 to nnode should be present.

The next *nelem* lines list the layer number and nodes for each element. They are arranged as:  $elem\_no\ mate\_id\ node\_1\ node\_2\ \dots$ 

where  $elem\_no$  is the number of element,  $mate\_id$  is an integer to indicate the material number of the element, and  $node\_i$  ( $i=1,2,\ldots$ ) are nodes belonging to this element. If nlayer is not equal to zero, then  $mate\_id$  should be replaced with  $layer\_id$  which will be defined later. Arrangement of  $elem\_no$  is not necessary to be consecutive, but all elements starting from 1 to nelem should be present. If the SG is meshed using regular elements (e.g., elements having the same dimension as the SG,

- 1D elements could have up to 5 nodes. If a node is not present in the element, the value is 0; see Figure 7.
- 2D elements could have up to 9 nodes. If a node is not present in the element, the value is 0. If the fourth node is zero, it is a triangular element; see Figure 8.

• 3D elements could have up to 20 nodes. If a node is not present in the element, the value is 0. If the fifth node is zero, it is a tetrahedral element; see Figure 9.

If trans\_flag is equal to 1, the next nelem lines list the orientation for each element. They are arranged as

```
elem\_no \ a_1 \ a_2 \ a_3 \ b_1 \ b_2 \ b_3 \ c_1 \ c_2 \ c_3
```

where  $elem\_no$  is the number of element,  $a_1, a_2, a_3$  are coordinates of point  $a, b_1, b_2, b_3$  are coordinates of point  $b, c_1, c_2, c_3$  are coordinates of point c. The local coordinate system for the element is defined by the three points a, b, c as described previously. Arrangement of  $elem\_no$  is not necessary to be consecutive, but all elements starting from 1 to nelem should be present.

If  $temp\_flag$  is equal to 1, the temperature distribution within the SG is not uniform, the next nnode lines list the corresponding nodal temperature. They are arranged as:

```
node\_no T
```

where  $node\_no$  is the nodal number and T is the corresponding temperature.

If *nslave* is not equal to 0, the next *nslave* lines list the slave nodes and corresponding master nodes periodic to the slave nodes. They are arranged as:

```
slave_node master_node
```

where *slave\_node* is an integer indicating the node slaved to the master node denoted by *master\_node*.

If *nlayer* is not equal to 0, the next *nlayer* lines list the definition for each layer. They are arranged as:

```
layer_id mate_id angle
```

where *layer\_id* is the layer number, *mate\_id* is the material type, and *angle* is a real number for the layup angle in degrees.

The next nmate blocks define the material properties. They are arranged as:

```
mat_id isotropy ntemp
```

where  $mat_{-}id$  is the material type, and isotropy is an integer to indicate whether the material is isotropic (0), orthotropic (1), or general anisotropic (2). The integer ntemp is number of material property sets according to different temperature followed by ntemp blocks of real numbers:

```
T_i \rho
```

```
const1 const2 ....
```

where  $T_i$ , i = 1, ..., ntemp is the temperature,  $\rho$  is the density, and the rest are material constants. For the convenience to compute secant values contained in thermal properties,  $T_1$  is used as the reference temperature and  $T_i$  must be arranged in an increasing fashion.

### 8.3 Conductivity

For **conduction analysis** (analysis=2), if the material is isotropic (isotropy=0), there is only one constant as the conductivity arranged as:

k

If isotropy=1 (orthotropic), there are three constants arranged as:  $k_{11}$   $k_{22}$   $k_{33}$  where  $k_{11}$ ,  $k_{22}$ ,  $k_{33}$  are conductivities along three principal directions.

If isotropy=2 (general anisotropic), there are six constants arranged as:  $k_{11}$   $k_{12}$   $k_{13}$   $k_{22}$   $k_{23}$   $k_{33}$ 

where  $k_{ij}$  are the components of the second-order conductivity tensor.

### 8.4 Elastic Properties

For all other analyses, we need to first provide elastic properties. if isotropy=0, there are two constants arranged as:

$$E - \nu$$

where E is the Young's modulus,  $\nu$  is the Poisson's ratio. Elasticity theory restricts that Poisson's ratio must be greater than -1.0 and less than 0.5 for linear, elastic, isotropic materials, although SwiftComp<sup>TM</sup> allows users to input values that are very close to those limits.

If isotropy=1, there are nine constants arranged as:

$$E_1$$
  $E_2$   $E_3$   $G_{12}$   $G_{13}$   $G_{23}$   $\nu_{12}$   $\nu_{13}$   $\nu_{23}$ 

including Young's moduli  $(E_1, E_2, \text{ and } E_3)$ , shear moduli  $(G_{12}, G_{13}, \text{ and } G_{23})$ , and Poisson's ratios  $(\nu_{12}, \nu_{13}, \text{ and } \nu_{23})$ . The convention of values is such that these values will be used to form the generalized Hooke's law for the orthotropic material in Eq. (5).

If isotropy=2, there are 21 constants arranged as:

These values are defined using the generalized Hooke's law given in Eq. (3). For orthotropic and general anisotropic materials, SwiftComp<sup>TM</sup> does not check the validity of the material inputs and it is the user's responsibility to make sure that the material properties satisfy the positive definiteness requirement of the stiffness matrix and compliance matrix found in a typical textbook on *Mechanics of Composites*.

### 8.5 CTE and Specific Heat

For thermally coupled analysis (analysis=1, 4, 6), if isotropy=0, there are two constants arranged as:

 $\alpha$   $c_{\epsilon}$ 

where  $\alpha$  is the CTE, and  $c_{\epsilon}$  is the specific heat.

If isotropy=1, there are four constants arranged as:

 $\alpha_{11}$   $\alpha_{22}$   $\alpha_{33}$   $c_{\epsilon}$ 

where  $\alpha_{11}, \alpha_{22}, \alpha_{33}$  are the CTEs along three principal directions.

If isotropy=2, there are seven constants arranged as:

 $\alpha_{11}$   $\alpha_{22}$   $\alpha_{33}$   $2\alpha_{23}$   $2\alpha_{13}$   $2\alpha_{12}$   $c_{\epsilon}$ 

where  $\alpha_{ij}$  are the components of the second-order CTE tensor.

### 8.6 Piezoelectric, Dielectric, and Pyroelectric Coefficients

If analysis=3,4,5,6, we then need to provide 18 piezoelectric coefficients arranged as:

The piezoelectric coefficients should be followed by dielectric properties. If isotropy=0, there is one constant for dielectric coefficient arranged as:

k

If isotropy=1, there are three constants arranged as:

 $k_{11}$   $k_{22}$   $k_{33}$ 

where  $k_{11}, k_{22}, k_{33}$  are the dielectric coefficients along three principal directions.

If isotropy=2, there are six constants arranged as:

 $k_{11}$   $k_{12}$   $k_{13}$   $k_{22}$   $k_{23}$ 

where  $k_{ij}$  denotes the second-order dielectric tensor.

If analysis=4,6, the above data should be followed by three pyroelectric coefficients arranged as:

 $p_1 p_2 p_3$ 

# 8.7 Piezomagnetic Coefficients, Magnetic Permeability, Electromagnetic and Pyromagnetic Coefficients

To carry out coupled piezoelectromagnetic analysis (analysis=5,6), we then need to provide another 18 piezomagnetic coefficients arranged as:

```
q_{11}
         q_{12}
                    q_{13}
                              q_{14}
                                        q_{15}
                                                  q_{16}
q_{21}
         q_{22}
                    q_{23}
                              q_{24}
                                        q_{25}
                                                  q_{26}
q_{31}
                              q_{34}
         q_{32}
                    q_{33}
                                        q_{35}
                                                  q_{36}
```

The piezomagnetic coefficients should be followed by magnetic permeability and electromagnetic coefficients. If isotropy=0, there are two constants arranged as:

 $\frac{\mu}{a}$ 

with  $\mu$  as the magnetic permeability, and a as the electromagnetic coefficient.

If isotropy=1, there are six constants arranged as:

```
\mu_{11} \mu_{22} \mu_{33} a_{11} a_{22} a_{33}
```

where  $\mu_{11}$ ,  $\mu_{22}$ ,  $\mu_{33}$  are the magnetic permeability along three principal directions, and  $a_{11}$   $a_{22}$   $a_{33}$  are the electromagnetic coefficients along three principal directions.

If isotropy=2, there are 12 constants arranged as:

```
\begin{array}{ccccc} \mu_{11} & \mu_{12} & \mu_{13} \\ & \mu_{22} & \mu_{23} \\ & & \mu_{33} \\ a_{11} & a_{12} & a_{13} \\ & a_{22} & a_{23} \\ & & a_{33} \end{array}
```

where  $\mu_{ij}$  denotes the second-order magnetic permeability tensor and  $a_{ij}$  denotes the second-order electromagnetic coupling tensor.

If analysis=6, the above data should be followed by three pyromagnetic coefficients arranged as:

```
m_1 m_2 m_3
```

To clarify the order of input material properties, if analysis=6 and isotropy=2, the material inputs should be arranged:

```
\alpha_{33}
                             2\alpha_{23} 2\alpha_{13} 2\alpha_{12} c_{\epsilon}
e_{11}
          e_{12}
                     e_{13}
                                e_{14}
                                           e_{15}
                                                     e_{16}
e_{21}
           e_{22}
                     e_{23}
                                e_{24}
                                           e_{25}
                                                      e_{26}
          e_{32}
                     e_{33}
                                e_{34}
e_{31}
                                           e_{35}
                                                      e_{36}
k_{11}
       k_{12} k_{13}
        k_{22} k_{23}
                  k_{33}
                  p_3
p_1
        p_2
          q_{12}
                     q_{13}
q_{11}
                                q_{14}
                                           q_{15}
                                                     q_{16}
q_{21}
           q_{22}
                     q_{23}
                                q_{24}
                                           q_{25}
                                                     q_{26}
          q_{32}
q_{31}
                     q_{33}
                                q_{34}
                                           q_{35}
                                                     q_{36}
\mu_{11} \mu_{12} \mu_{13}
          \mu_{22} \mu_{23}
                   \mu_{33}
          a_{12}
                     a_{13}
           a_{22}
                     a_{23}
                      a_{33}
m_1
          m_2
                     m_3
```

The material constants could be expressed in the problem coordinate system  $y_1, y_2, y_3$ . However, it is usually more convenient and simpler to provide these constants in the material coordinate system. If it is expressed in the material coordinate system, SwiftComp<sup>TM</sup> will perform the necessary transformations. The input quantities should be properly scaled as discussed previously for multiphysics modeling. It is also emphasized that if the users uses an arrangement of stresses and strains are different from what SwiftComp<sup>TM</sup> uses, proper re-arrangement of the material properties is needed.

The following line is used to input  $\omega$ , the volume of the domain spanned by the remaining coordinates in the macroscopic structural model. For 3D structural models,  $\omega$  will be the volume of the homogenized material including both the volume of the material and the volume of possible voids in the SG.  $\omega$  can be computed by any mesh generator. For regular SG such as cubes, it can be easily calculated by hand. Of course, for 1D SGs, the volume is the length and for 2D SGs, the volume is the area. For plate/shell models,  $\omega$  will be the area spanned by  $y_1$  and  $y_2$  for 3D SGs, the length along  $y_2$  for 2D SGs and 1.0 for 1D SGs. For beam models,  $\omega$  will be the length along  $y_1$  for 3D SGs and 1.0 for 2D SGs.

Till now, we have prepared all the inputs necessary for the homogenization run.

# 9 SwiftComp $^{TM}$ Inputs for Dehomogenization Run

For dehomogenization, the user needs to provide additional information obtained from the macroscopic analysis including the macroscopic primary field (such as temperature for heat conduction or displacement for the elastic analysis) and the generalized strain vector according to Eq. (28). This information are provided in a text file corresponding to the input file name with extension qlb.

For example if the input file is *test.sc*, one should also prepare a file called *test.sc.glb* for dehomogenization holding the data as described below.

If analysis=0, then the macroscopic displacements, rotations, and mechanical strains are to be provided to compute the local displacement/strain/stress fields. The data are arranged as:

where  $v_1$ ,  $v_2$ , and  $v_3$  are the macro displacements,  $C_{ij}$  are macro rotations, and  $\bar{\epsilon}$  contains the macro generalized strains.  $C_{ij}$  is defined such that  $B_i = C_{ij}b_j$  where  $b_j$  is the base vector for undeformed configuration and  $B_i$  is the base vector for the deformed configuration. For example, for a linear analysis of 3D structures,

$$C_{ij} = \begin{bmatrix} 1 + u_{1,1} & u_{2,1} & u_{3,1} \\ u_{1,2} & 1 + u_{2,2} & u_{3,2} \\ u_{1,3} & u_{2,3} & 1 + u_{3,3} \end{bmatrix}$$
(37)

For linear analysis of plates/shells using the classical plate model (Kirchhoff-Love model),

$$C_{ij} = \begin{bmatrix} 1 + u_{1,1} & u_{2,1} & u_{3,1} \\ u_{1,2} & 1 + u_{2,2} & u_{3,2} \\ -u_{3,1} & -u_{3,2} & 1 + u_{1,1} + u_{2,2} \end{bmatrix}$$
(38)

For linear analysis of beams using the classical beam model (Euler-Bernoulli model),

$$C_{ij} = \begin{bmatrix} 1 & u_2' & u_3' \\ -u_2' & 1 & \theta_1 \\ -u_3' & -\theta_1 & 1 \end{bmatrix}$$
(39)

where  $u_i$  are the global displacements and  $\theta_1$  is the twist angle.

Here  $id_1$  indicates whether generalized stresses or generalized strains are used for dehomogenization run. If it is equal to 0, generalized stresses are used as inputs; if it is equal to 1, generalized strains are used as inputs. For 3D structures  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \epsilon_{22} & \epsilon_{33} & 2\epsilon_{23} & 2\epsilon_{12} \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{33} & \sigma_{23} & \sigma_{13} & \sigma_{12} \end{bmatrix}^T$ . For Kirchhoff-Love plate/shell model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \epsilon_{22} & 2\epsilon_{12} & \kappa_{11} & \kappa_{22} & 2\kappa_{12} \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} N_{11} & N_{22} & N_{12} & M_{11} & M_{22} & M_{12} \end{bmatrix}^T$ . For Reissner-Mindlin plate/shell model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \epsilon_{22} & 2\epsilon_{12} & \kappa_{11} & \kappa_{22} & 2\kappa_{12} & \gamma_{13} \\ \bar{\sigma} = \begin{bmatrix} N_{11} & N_{22} & N_{12} & M_{11} & M_{22} & M_{12} & N_{13} & N_{23} \end{bmatrix}^T$ . For Euler-Bernoulli beam model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \kappa_{11} & \kappa_{12} & \kappa_{13} \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} F_1 & M_1 & M_2 & M_3 \end{bmatrix}^T$ . For Timoshenko model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \gamma_{12} & \gamma_{13} & \kappa_{11} & \kappa_{12} & \kappa_{13} \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} F_1 & F_2 & F_3 & M_1 & M_2 & M_3 \end{bmatrix}^T$ .

If analysis=1, we need to provide an additional data for the macroscopic temperature difference  $T_m$  to compute the thermoelastic effects.  $T_m$  is the difference between the current macroscopic temperature with respect to the reference temperature  $T_1$ . The data are arranged as:

$$v_1$$
  $v_2$   $v_3$   $C_{11}$   $C_{12}$   $C_{13}$ 

```
C_{21} C_{22} C_{23} C_{31} C_{32} C_{33} id_1 \bar{\epsilon} or \bar{\sigma} T_m

If analysis=2, we need to provide the following four values, arranged as T id_1 T_{,1} T_{,2} T_{,3} or -q_1 -q_2 -q_3 where T_{,i} are the gradient of the macroscopic temperature, and q_i are the macroscopic heat flux.
```

If analysis=3 or 4, we need to provide the following data for dehomogenization, which are arranged as:

```
v_1 v_2 v_3 \phi^*
C_{11} C_{12} C_{13}
C_{21} C_{22} C_{23}
C_{31} C_{32} C_{33}
id_1
\bar{\epsilon} or \bar{\sigma}
T_m
```

with  $\phi^*$  as the scaled electric potential,  $\bar{\epsilon}$  as the macro generalized strains, and  $\bar{\sigma}$  as the macro generalized stresses. For 3D structures  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \epsilon_{22} & \epsilon_{33} & 2\epsilon_{23} & 2\epsilon_{13} & 2\epsilon_{12} & -E_1^* & -E_2^* & -E_3^* \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{33} & \sigma_{23} & \sigma_{13} & \sigma_{12} & D_1 & D_2 & D_3 \end{bmatrix}^T$ . For Kirchhoff-Love plate/shell model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \epsilon_{22} & 2\epsilon_{12} & \kappa_{11} & \kappa_{22} & 2\kappa_{12} & -E_1^* & -E_2^* \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} N_{11} & N_{22} & N_{12} & M_{11} & M_{22} & M_{12} & D_1 & D_2 \end{bmatrix}^T$ . For Reissner-Mindlin plate/shell model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \epsilon_{22} & 2\epsilon_{12} & \kappa_{11} & \kappa_{22} & 2\kappa_{12} & \gamma_{13} & \gamma_{23} & -E_1^* & -E_2^* \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} N_{11} & N_{22} & N_{12} & M_{11} & M_{22} & M_{12} & N_{13} & N_{23} & D_1 & D_2 \end{bmatrix}^T$ . For Euler-Bernoulli beam model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \kappa_{11} & \kappa_{12} & \kappa_{13} & -E_1^* \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} F_1 & M_1 & M_2 & M_3 & D_1 \end{bmatrix}^T$ . For Timoshenko model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \gamma_{12} & \gamma_{13} & \kappa_{11} & \kappa_{12} & \kappa_{13} & D_1 \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} F_1 & F_2 & F_3 & M_1 & M_2 & M_3 & D_1 \end{bmatrix}^T$ . Here  $\phi_{,i}^* = -E_i^*$ . If analysis is 3, the macroscopic temperature difference  $T_m$  does not exist.

If analysis = 5 or 6, we need to the following data which are arranged as:

```
v_1 v_2 v_3 \phi^* \psi^* C_{11} C_{12} C_{13} C_{21} C_{22} C_{23} C_{31} C_{32} C_{33} id_1 \bar{\epsilon} or \bar{\sigma}
```

with  $\psi^*$  as the scaled magnetic potential,  $\bar{\epsilon}$  as the macro generalized strains, and  $\bar{\sigma}$  as the macro generalized stresses.

For 3D structures  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \epsilon_{22} & \epsilon_{33} & 2\epsilon_{23} & 2\epsilon_{13} & 2\epsilon_{12} & -E_1^* & -E_2^* & -E_3^* & -H_1^* & -H_2^* & -H_3^* \end{bmatrix}^T$ ,  $\bar{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{33} & \sigma_{23} & \sigma_{13} & \sigma_{12} & D_1 & D_2 & D_3 & B_1 & B_2 & B_3 \end{bmatrix}^T$ . For Kirchhoff-Love plate/shell model,  $\bar{\epsilon} = \begin{bmatrix} \epsilon_{11} & \epsilon_{22} & 2\epsilon_{12} & \kappa_{11} & \kappa_{22} & 2\kappa_{12} & -E_1^* & -E_2^* & -H_1^* & -H_2^* \end{bmatrix}^T$ ,

### 10 SwiftComp<sup>TM</sup> Inputs for Failure Analysis

A corresponding homogenization analysis must be run before carrying out any failure analysis.

For failure analysis (including initial failure strength, initial failure index/strength ratio, and initial failure envelope), the \*.glb file will be used to store the data needed for failure analysis instead. First, additional material properties are needed for each material at each given temperature including a failure criterion and corresponding strength constants. Three lines will be inserted and the inputs needed for failure analyses should be arranged as:

```
failure\_criterion num\_of\_constants \\ l_c
```

 $const_1 \ const_2 \ const_3 \ \dots$ 

failure\_criterion is an integer identifier for the failure criterion.  $num\_of\_constants$  indicates the number of strength constants needed for the corresponding failure criterion.  $l_c$  is a real number indicating the characteristic length used in the nonlocal approach for initial failure analysis. If  $l_c$  is equal to zero, the local approach based on element averaged values will be used.  $const_1\ const_2\ const_3\dots$  are the corresponding strength constants. It is noted that this block of data should be corresponding to the material block in the main input file. In other words, for each material with  $mat\_id$ , we need to provide such information for each temperature.

failure\_criterion can be equal to 1, 2, 3, 4, 5, and another number greater than 10. For isotropic material, 1 is max principal stress criterion, 2 is max principal strain criterion, 3 is max shear stress criterion (also commonly called Tresca criterion), 4 max shear strain criterion, and 5 is Mises criterion. For anisotropic materials, 1 is max stress criterion for anisotropic materials, 2 is max strain criterion for anisotropic materials, 3 is Tsai-Hill criterion, 4 is Tsai-Wu criterion and 5 is Hashin criterion. 11 and larger indicates a user-defined failure criterion. If failure\_criterion is equal to 1, 2, 3, 4, 5,  $num\_of\_constants$  is not used. If it is a user-defined failure criterion, then  $num\_of\_constants$  will be used to input the right number of strength constants. It is assumed that the number of strength constants will not be greater than 9 for a material. If the material is isotropic, the failure criterion and corresponding strength constants are defined as follows.

- If  $failure\_criterion$  is 1, the max principal stress criterion is used and two strength constants are needed: one for tensile strength (X) and one for compressive strength (X'), arranged as X, X'.
- If  $failure\_criterion$  is 2, the max principal strain criterion is used and two strength constants are needed: one for tensile strength  $(X_{\epsilon})$  and one for compressive strength  $(X'_{\epsilon})$ , arranged as  $X_{\epsilon}, X'_{\epsilon}$ .

- If failure\_criterion is 3, the max shear stress criterion (aka Tresca criterion) is used and one shear strength constant (S) is needed.
- If  $failure\_criterion$  is 4, the max shear strain criterion is used and one shear strength constant  $(S_{\epsilon})$  is needed.
- If failure\_criterion is 5, the Mises criterion is used and one strength constant (X) is needed.

If the material is **not isotropic** (transversely isotropic, orthotropic or general anisotropic), the failure criterion and corresponding strength constants are defined as follows.

- If  $failure\_criterion$  is 1, the max stress criterion is used and nine strength constants are needed: three for tensile strengths (X,Y,Z) in three directions, three for compressive strengths (X',Y',Z') in three directions, and three for shear strengths (R,T,S) in three principal planes, arranged as X,Y,Z,X',Y',Z',R,T,S.
- If failure\_criterion is 2, the max strain criterion is used and nine strength constants are needed: three for tensile strengths  $(X_{\epsilon}, Y_{\epsilon}, Z_{\epsilon})$  in three directions and three for compressive strengths  $(X'_{\epsilon}, Y'_{\epsilon}, Z'_{\epsilon})$  in three directions, and three for shear strengths  $(R_{\epsilon}, T_{\epsilon}, S_{\epsilon})$  in three principal planes, arranged as  $X_{\epsilon}, Y_{\epsilon}, Z_{\epsilon}, X'_{\epsilon}, Y'_{\epsilon}, Z'_{\epsilon}, R_{\epsilon}, T_{\epsilon}, S_{\epsilon}$ .
- If  $failure\_criterion$  is 3, the Tsai-Hill criterion is used and six strength constants are needed: three for normal strengths in three directions and three for shear strengths in three principal planes, arranged as X, Y, Z, R, T, S.
- If failure\_criterion is 4, the Tsai-Wu criterion is used and nine strength constants are needed: three for tensile strengths (X,Y,Z) and three for compressive strengths (X',Y',Z') in three directions and three for shear strengths (R,T,S) in three principal planes, arranged as X,Y,Z,X',Y',Z',R,T,S.
- If  $failure\_criterion$  is 5, the Hashin criterion is used and six strength constants are needed: two for tensile strengths (X,Y) and two for compressive strengths (X',Y') in two directions and two for shear strengths (R,S) in two principal planes, arranged as X,Y,X',Y',R,S.

It is noted that for failure analysis, general anisotropic materials are also approximated using orthotropic materials due to limited number of strength constants. In SwiftComp, both the tensile strengths and compressive strengths are expressed using positive numbers. In other words, in the uniaxial compressive test along  $y_1$  direction,  $\sigma_{11} = -X'$  when material fails.

After the material block for strength parameters, we need to provide the following line in the \*.glb file containing one integer.

 $id_1$ 

Here  $id_1$  indicates whether the strength is expressed in terms of generalized stresses or generalized strains. If it is equal to 0, the strength is expressed in terms of generalized stresses; if it is equal to 1, it is expressed in terms of generalized strains.

For failure envelope analysis, we need to provide the following line in the \*.glb file containing three integers.

 $istr_1$   $istr_2$  idiv

Here  $istr_1$  and  $istr_2$  indicate the two load directions that one would like to predict a failure envelope for. The values could be 1, 2, 3, 4,..., corresponding to the arrangement of the generalized stresses (if  $id_1 = 0$ ) or generalized strains (if  $id_1 = 1$ ). For example for the 3D model, the stress/strain are arranged in the order of 11, 22, 33, 23, 13, 12. If we want to draw a  $\bar{\sigma}_{22} - \bar{\sigma}_{13}$  failure envelope, we will have  $istr_1 = 2$ ,  $istr_2 = 5$ . The integer idiv indicates how many divisions along one direction one would like to use for searching for failure envelope points. The total failure envelope points will be about  $4 \times idiv$ . Although one is free to use any number for idiv, it is recommend to use 10 for a balance between efficiency and accuracy in describing the failure envelope.

For failure index analysis, we need to provide the following line in the \*.glb file containing n real numbers with n equal to the total number of generalized stresses or generalized strains.

$$str_1$$
  $str_2$   $str_3$  ...  $str_n$ 

Here  $str_1, str_2, ..., str_n$  indicate the given loads used to compute the strength ratio and the failure index. These values can be given in terms of generalized stresses or generalized strains depending on whether the required strength outputs are in generalized stresses ( $id_1 = 0$ ) or generalized strains ( $id_1 = 1$ ).

Both input files, input\_file\_name and input\_file\_name.glb, should be ended with a blank line to avoid any possible incompatibility of different computer operating systems. The input file can be given any name as long as the total number of the characters of the name including extension is not more than 256. For the convenience of the user to identify mistakes in the input file, all the inputs are echoed in a file named input\_file\_name.ech. Error messages are also written at the end of input\_file\_name.ech and on the output screen.

## 11 SwiftComp<sup>TM</sup> Outputs

Effective properties computed by SwiftComp<sup>TM</sup> are stored in *input\_file\_name.k*, including effective stiffness matrix corresponding to Eq. (31), effective flexibility matrix (inverse of stiffness matrix), effective thermal coefficients including CTEs, specific heat, pyroelectric coefficients, and pyromagnetic coefficients.

If the material can be approximated as orthotropic material, engineering constants corresponding to the elastic stiffness matrix is also provided among the outputs.

Regarding the effective specific heat, there are two contributions  $\langle C_v \rangle$  and  $F_{eff}$  and the effective specific heat can be calculated as

$$\bar{C}_{\epsilon} = \langle C_v \rangle - TF_{eff}$$

with T as the current temperature  $T = T_1 + T_m$ .

The effective density of the SG is also listed as one output.

In the outputs of dehomogenization, the primary local field such as the displacement field for elastic analysis or the temperature field for conduction analysis is reported at each node. However, other fields calculated based on gradients from the primary local field such as stresses and strains are usually more accurate if reported at Gaussian integration points. However, because nodal values are more convenient for postprocessing of the results, only nodal values are reported. If you need Gaussian values, please contact the author.

The local 3D displacement results obtained through dehomogenization are stored in *input\_file\_name.u*. The values are listed for each node identified by its location as:

```
node\_no \ u_1 \ u_2 \ u_3
```

where  $u_i$  are the local 3D displacements at this node. Note if analysis=2, the outputs in this file are the local temperature for each node instead.

```
If analysis=3, 4, the outputs will be node\_no\ u_1\ u_2\ u_3\ \phi^* with \phi^* as the scaled electric potential.
```

```
If analysis=5, \theta, the outputs will be node\_no\ u_1\ u_2\ u_3\ \phi^*\ \psi^* with \psi^* as the scaled magnetic potential.
```

The local 3D strain/stress results at nodes obtained through dehomogenization are stored in *input\_file\_name.sn*. These values are identified by its location as:

```
y_1 y_2 y_3 \epsilon_{11} \epsilon_{22} \epsilon_{33} 2\epsilon_{23} 2\epsilon_{12} \sigma_{11} \sigma_{22} \sigma_{33} \sigma_{23} \sigma_{13} \sigma_{12} where \epsilon_{ij} and \sigma_{ij} are the components of the local 3D strain tensor and 3D stress tensor, respectively, at the node. Note if analysis=2, the outputs in this file are instead the local temperature gradient and heat flux instead arranged as
```

```
y_1 \ y_2 \ y_3 \ T_{,1} \ T_{,2} \ T_{,3} \ q_1 \ q_2 \ q_3.
```

```
If analysis=3, 4, the outputs will be y_1 \ y_2 \ y_3 \ \epsilon_{11} \ \epsilon_{22} \ \epsilon_{33} \ 2\epsilon_{23} \ 2\epsilon_{13} \ 2\epsilon_{12} \ -E_1^* \ -E_2^* \ -E_3^* \ \sigma_{11} \ \sigma_{22} \ \sigma_{33} \ \sigma_{23} \ \sigma_{13} \ \sigma_{12} \ D_1 \ D_2 \ D_3
```

If analysis=5, 6, the outputs will be

```
y_1 \ y_2 \ y_3 \ \epsilon_{11} \ \epsilon_{22} \ \epsilon_{33} \ 2\epsilon_{23} \ 2\epsilon_{13} \ 2\epsilon_{12} \ -E_1^* \ -E_2^* \ -E_3^* \ -H_1^* \ -H_2^* \ -H_3^* \ \sigma_{11} \ \sigma_{22} \ \sigma_{33} \ \sigma_{23} \ \sigma_{13} \ \sigma_{12} \ D_1 \ D_2 \ D_3 \ B_1 \ B_2 \ B_3.
```

If the local results are desired to be output in Gmsh format (arg3=LG or LAG), the recovered 3D strain/stress results at nodal points are stored in input\_file\_name.sn. This file contains a block for each generalized strain or stress component as follows:

```
elem_no nodes nodal_value
```

where *elem\_no* is the corresponding element number, *nodes* is the total number of nodes in this element, and *nodal\_values* is an array holding *nodes* nodal values of the strain or strain component. Each block contains *nelem* lines and blocks are separated by a blank line. For example, if *analysis=5,6*, there will be 24 blocks of data arranged according to the order first for the gener-

alized strains, then for the generalized stresses according to SwiftComp<sup>TM</sup> convention specified in Eqs. (28) and (29).

The above local 3D strain/stress results are expressed in the problem coordinate system. Sometimes it is more convenient to have strain/stress values expressed in the material coordinate system. These values at nodal points are stored in the file <code>input\_file\_name.snm</code>.

The failure analysis results are stored in the file <code>input\_file\_name.fi</code>, the content of which depends on the type of analysis. For failure <code>index analysis</code>, the failure index and strength ratio for each element are stored in the file <code>input\_file\_name.fi</code> with the first number is an integer indicating the element number and the following two numbers are the initial failure index and the initial strength ratio for each element under given loads. For initial strength analysis, this file stores the initial failure strengths in both tensile and compressive directions. For failure envelope analysis, this file stores the failure envelope points with the first number being the number of the failure point, the two trailing read numbers being the values for corresponding two given directions for predicting the failure envelope.

All these output files are in pure text format and can be opened and edited by any text editor.

### 12 SwiftComp<sup>TM</sup> Maintenance and Tech Support

SwiftComp<sup>TM</sup>is available in the cloud on cdmHUB and users can execute the code within a web browser. A group named *Prof. Yu's Research Group In the Cloud* is specifically set up on cdmHUB for information exchange related with SwiftComp<sup>TM</sup>. *Users are highly encouraged to join the group through http://cdmhub.org/groups/yugroup* to receive most recent news of SwiftComp<sup>TM</sup>, ask questions, and share with others. For the sake of efficiency and reusability, **please post your questions in the group.** A page of SwiftComp<sup>TM</sup> FAQ will be constantly updated in the group. Before you ask questions, please do the following:

- 1. Read this manual carefully, if you have not done so;
- 2. Check the error message at the end of input\_file\_name.ech;
- 3. Make sure that you have provided the right input data through *input\_file\_name.ech*, which is your input file understood by SwiftComp<sup>TM</sup>;
- 4. Check the SwiftComp<sup>TM</sup> FAQ page in the group;
- 5. Post your question in the discussion section of the group.

### 13 Epilogue

Although still in its early development age, SwiftComp<sup>TM</sup> has demonstrated great potential for multiscale constitutive modeling of materials and structures. Its accuracy has been extensively verified by its developers and users. The performance and robustness of code will be continuously

improved based on feedback from its users throughout the world. Although SwiftComp<sup>TM</sup> has been designed in such a way that end users do not have to fully understand its theoretical foundation (the details of which are spelled out in SwiftComp<sup>TM</sup> related publications), further questions are inevitable because SwiftComp<sup>TM</sup> represents a unique unified approach for modeling composite structures and materials which is drastically different from most conventional micromechanics and structural mechanics approaches. Nevertheless, it should be clear that SwiftComp<sup>TM</sup> is emerging as a general-purpose computational tool for engineers to perform multiscale constitutive modeling of composites.

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