Integrated Prediction Of Macroscopic Properties Of Composites Based On Finite Element Computational Micromechanics

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Abstract

A novel technique to automatically generate macroscopic properties of composites is presented. This integral technique was developed based on the method of finite element computation micromechanics (FECM). We used the advanced pre- and post-processing software, MSC.PATRAN, as the platform for the establishment of representative volume element (RVE) library. By the processes of Boolean operations of RVE modeling and the matching of finite element meshes at the bi-constituents interface, the automatic parametric modeling of RVE were implemented. Through changing the PATRAN record file, *.ses file, to a modeling function by using PATRAN command language (PCL), the integral design had been carried out. At present, the RVE Library included four different patterns. According to the various micromechanics methods, the calculating program of the micromechanics were also integrated into the platform by PCL, then the macroscopic properties of composites were gained.

Lastly, macroscopic elastic properties of unidirectional composites were predicted as the example to demonstrate the integrated system.

1 Introduction

Finite element computational micromechanics (FECM) have been the primary approaches to predict the macroscopic properties as the geometrical configuration of composite structures become more and more complicated [1]. The key of the FECM is to establish the proper representative volume element (RVE). So far, many RVE have been established for various composites and used to calculate the effective elastic modulus, rupture strength, thermal properties, etc. according to some research achievements. Furthermore, some achievements (primarily in linear elastic analysis) are mature relatively and can be absolutely used in engineering [2]. Recent advances in computational speed and powerful FEM tool have resulted in the ability to realize the integrated design of macroscopic properties prediction of composites. W.Sun [3] constructed the CAD model of RVE and calculated the stress field of it by Pro/E and Pro/M. Just as the destination of finite element calculation, it was not getting the accurate predictive value, but verifying the seamless integration between CAD and CAE. D.Brown [4] developed the parameterized automatic modeling system using the Open Language function of I-deas. But that system did not integrate the calculation program to predict the properties of composites.

In this paper, advanced pre- and post-processing software, MSC.PATRAN, is used as the platform in the RVE library establishment and calculating program integration. Lastly, macroscopic elastic properties of unidirectional composite are used as the example to demonstrate the integrated system of macroscopic properties prediction of composites.

2 Basic calculating method of FECM

The essential of FECM in simulating the mechanical behavior of composites is constructing the RVE based on the microstructure under phase and boundary conditions, establishing the relationship between local and macro-average field values, and finally getting the macroscopic mechanical response. It is pointed out that, the "quantitative" relation between material microstructure and effective modulus, which can't be obtained by the analytical method of micromechanics [5], can be gotten by the FECM.

According to the basic assumption of micromechanics, the field values of mechanics are continuous, so the all of the phase behaviors can be described by the continuous constitutive relationship. The macroscopic deformation can be gotten by the solution of the governing and energy balance equations under initial values and boundary conditions.

Elastic tensor $\mathbf{C}$ and compliance tensor $\mathbf{S}$ of phase are the periodic function of the position. Periodic solution can be expressed as,

$$\boldsymbol{\sigma}(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x}+\mathbf{d}),\ \boldsymbol{\varepsilon}(\mathbf{x}) = \boldsymbol{\varepsilon}(\mathbf{x}+\mathbf{d}) \tag{1}$$

$$\mathbf{d} = \sum_{i=1}^{3} 2m_i a_i \mathbf{e}_i \tag{2}$$

m_i（i=1,2,3）is arbitrary integer and $a = (a_i \mathbf{e}_i)$ is edge vectors of solid element. If average strain and stress express as $\langle \boldsymbol{\varepsilon} \rangle$ and $\langle \boldsymbol{\sigma} \rangle$, under given boundary condition $\mathbf{u}^0\big|_{\partial V} = \boldsymbol{\varepsilon}^0 \cdot \mathbf{x}$, the integral can be dispersed as

$$\begin{aligned}\langle \boldsymbol{\varepsilon} \rangle &= \frac{1}{V}\int_V \boldsymbol{\varepsilon}(\mathbf{x})dV \\ &= \frac{1}{V}\int_{\partial V} \frac{1}{2}\left(\mathbf{n}\cdot\mathbf{u}^0 + \mathbf{u}^0\cdot\mathbf{n}\right)ds = \sum_m \sum_n \varepsilon_{ij}^{mn} dV^{mn}\end{aligned} \tag{3}$$

$$\begin{aligned}\langle \boldsymbol{\sigma} \rangle &= \frac{1}{V}\int_V \boldsymbol{\sigma}(\mathbf{x})dV \\ &= \frac{1}{V}\int_V C(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x})dV = \sum_m \sum_n \sigma_{ij}^{mn} dV^{mn}\end{aligned} \tag{4}$$

n is sum of the gauss points and m is sum of the elements. In this paper, we can get the $\langle \boldsymbol{\varepsilon} \rangle$ and $\langle \boldsymbol{\sigma} \rangle$ by the finite element software. Macroscopic elastic properties can be decided by the anisotropic constitutive relationship.

$$\langle \boldsymbol{\sigma} \rangle = \mathbf{C}^* \langle \boldsymbol{\varepsilon} \rangle,\ \langle \boldsymbol{\varepsilon} \rangle = \mathbf{S}^* \langle \boldsymbol{\sigma} \rangle \tag{5}$$

$\mathbf{C}^*, \mathbf{S}^*$ is effective elastic and compliance tensor respectively.

Micro-local and macro-average field values are introduced using simple relationships, including the basic mathematical equations, constitutive relationship and boundary conditions, etc. The micro-local field values can be gotten correctly by establishing the RVE which can reflect the microstructure of composites accurate, furthermore, the macroscopic mechanical response can be obtained.

3 Parameterized finite element modeling of RVE

Constructing RVE plays a central role in the prediction of macroscopic properties of composites. Because the either one parameter changing also make the whole of RVE change, the repeated modeling work in constructing RVE become cost-consuming and tedious. Several attempts have been made in literatures [3,4,6] to form a unified procedure to determine the RVE. Advanced CAE software, MSC.PATRAN 2005-R2 by parametric technology, is used in the automatic generation of RVE models.

3.1 RVE establishment

In the modeling construction, the boolean operation algorithm is applied to manipulate fiber bundle and matrix topological elements and to construct the heterogeneous composites RVE. Example of using the technique to construct RVE representing unidirectional composite and 3D 4-directional composite are given in Fig.1.

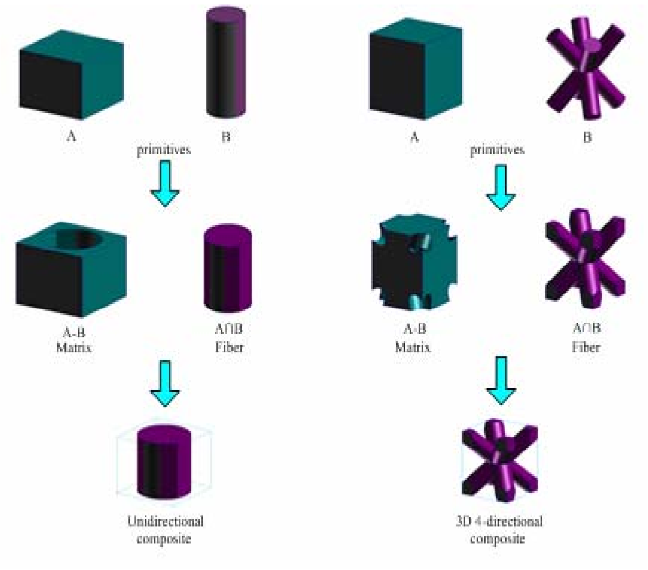

Fig.1. Boolean operations of RVE modeling

Interference checking reveals that all surfaces are "just touching", i.e. there is no overlapping or gaps in the model. This means that there is face-to-face contact over adjoining surfaces of adjacent solids. This is an important requirement of the RVE model which is used for downstream analysis purposes.

After generating the "assembly" of the RVE by PATRAN geometric modeling module, finite element meshing is generated through PATRAN solid meshing function for fiber bundle and matrix. To match meshes at the bi-material interface is a basic requirement in order to successfully conduct finite-element analysis for heterogeneous material structure. Often times, conventional finite element tool fails to generate finite-element meshes to match at the material interface, particularly in the analysis of composites with i.e. complex 2D or 3D textile architectures. The 2005-R2 version of MSC.PATRAN provides the powerful solid meshing tool (Assembly Parameters->Match Parasolid Faces function) to guarantee generating meshes to automatically match at the fiber bundle and matrix interfaces.

All of the operations of modeling the RVE in PATRAN have been recorded in the *.ses file. In order to automatically generate the RVE, recording a correct and succinct process of constructing the RVE in the *.ses file is done as the important step. Through modifying the record file, *.ses file, to the modeling function by PCL, the automatic modeling procedure of RVE is carried out.

3.2 Input parameters of RVE

The modeling parameters mainly include geometric parameters and physical parameters. The geometric parameters determine the configuration of RVE, such as fiber bundle volume fraction, braided angle, tow cross-sectional shape, filament diameter, number of filament, etc. The physical parameters determine the properties of RVE. So far, most of the RVE consist of matrix and fiber bundles. Few of it also include interfacial layer. It is pointed out that, in this paper, all of RVE don't contain the interfacial layer. According to the current research, the properties of matrix and interfacial layer are often defined as isotropic material and the property of fiber bundle is often defined as transversely isotropic or orthotropic material.

In PATRAN, parameterized modeling of RVE can be realized by means of setting the processing parametric values as the variables. The user can access the program to input the parameters via a graphical user interface (GUI) or via command line and ASCII-files. This paper, the GUI is developed and integrated in the PATRAN environment.

3.3 RVE library establishment

With the increase of 2D and 3D braided composites application, the former database which consist mainly of properties of unidirectional and laminate composites have been already not applicable. At present, because of involving numerous parameters and not yet standardization of technology, establishing braided composites database is infeasible. Parameterized finite element modeling of RVE is provided a new thought for structure analysis of composites. The customization design of GUI of modeling RVE is developed as the RVE library where the several RVE are classified and integrated in the PATRAN environment as the menu by using PCL too. The RVE library provides the approach to user like a consumer in the supermarket who can select the proper RVE to help the design and analysis of composite structure. The relative regular procedure of development supplies the good expansibility for RVE library.

Now, the RVE Library includes four different pattern RVE of composites, such as unidirectional composite's RVE, 2D plain weave composite's RVE, 3D 4-directional composite's "*"-type RVE and 3D 4-directional composite's winding-type RVE (Fig.2). According to the RVE, we initially divided the RVE of composites into three classifications including unidirectional composite, 2D composite and 3D composite.

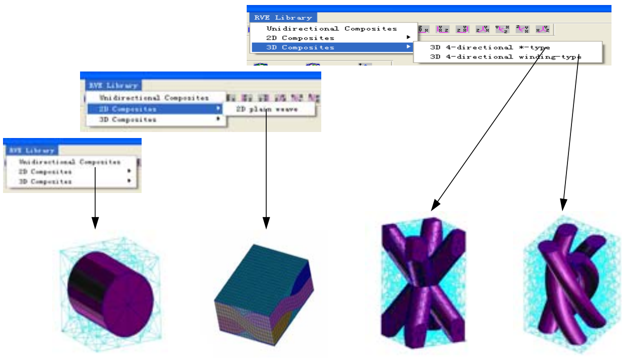

Fig.2. Four established RVE

4 Integrated prediction of macroscopic properties

The finite element model of RVE is provided by RVE Library. In order to automatically predict the macroscopic properties of composites, corresponding calculating program of micromechanics require to be integrated in the PATRAN environment. The processing flowchart of analysis of RVE and calculating program integration is shown in Fig.3.

The result of finite element analysis of RVE is the input of the calculating program according to the FECM. For the RVE, the different macroscopic properties of composites are mainly determined by the setting of different boundary conditions. Several relative research achievements have been reported. The linear elastic analysis of the micromechanics has been developed more maturely, so currently the finite element analysis of RVE is focused on this solution type. The stress field values or temperature field values of the RVE are calculated by MSC.NASTRAN. The input data are filtrated and disposed from the field data. All of operations are customized by PCL and are executed in the background.

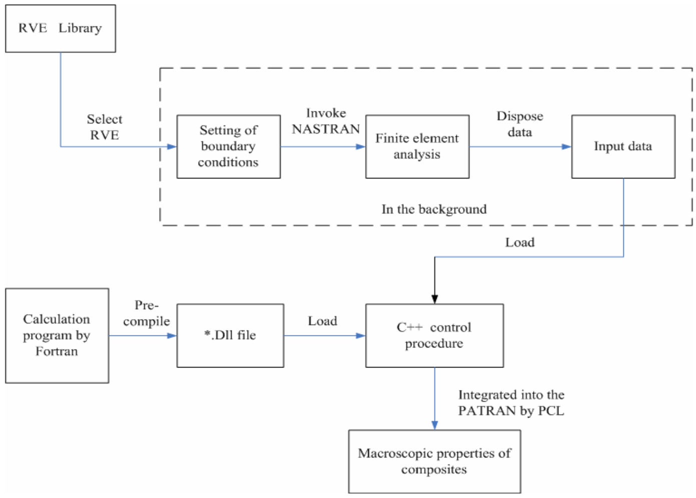

Fig.3. The processing flowchart of analysis of RVE and calculating program integration

The calculating program is developed based on the micromechanics of composites. All of calculating program is pre-complied to be the dynamic-link library (*.dll) file by FORTRAN in order to improve the precision of calculation and portability. The PCL functions are imbedded in C++ control program which can directly invoke the PCL functions of PATRAN. The input data of finite element analysis of RVE is read using the function of C++. In the end, the C++ program is compiled and integrated in the PATRAN by PCL, and the prediction of macroscopic properties of composites is easily generated by clicking the "Calculate" menu.

5 Example

For demonstrating the integrated system of macroscopic properties prediction of composites, macroscopic elastic properties prediction of unidirectional composite are presented in Fig.4.

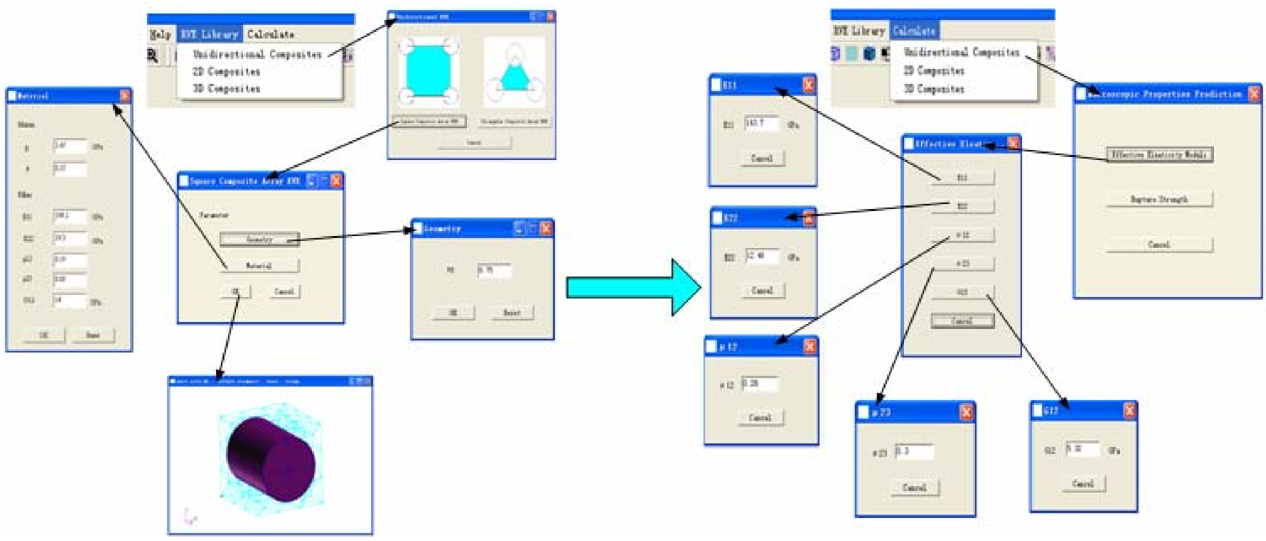

Fig.4. Integrated system of macroscopic elastic properties prediction of unidirectional composite

According to the numerical example of reference [7], the input of geometrical parameter is only the fiber bundle volume fraction $V_f = 0.75$; Matrix is defined as isotropic material and has two independent parameters; Fiber bundle is regarded as transversely isotropic material and has five independent parameters. The properties of constituents are as follows:

Table 1 The modulus of matrix and fiber bundle

Material	E_{11} / (GPa)	E_{22} / (GPa)	ν_{12}	ν_{23}	G_{12} / (GPa)
Graphite fiber Bundle	199.2	19.3	0.19	0.08	14
Epoxy Matrix	3.45	3.45	0.35	0.35	1.28

The finite element analysis of RVE is executed in the background of PATRAN and the calculating processes are also invisible in the platform. The unidirectional composite is also regarded as the transversely isotropic material. Because the different modulus have different setting of boundary conditions of RVE, calculating the each modulus need to do the independent finite element analysis of RVE. The effective elastic modulus can be gotten one by one. Comparing predictive values and experimental values, shown in Table 2. We can see that the calculating values are within the accuracy limits of engineering permitting.

Table 2 Comparing predictive values and experimental values

	E_{11} / (GPa)	E_{22} / (GPa)	ν_{12}	ν_{23}	G_{12} / (GPa)
Experiment	144.8	11.73	0.23	0.3	5.52
Calculation	143.7	12.46	0.26	0.30	5.32

6 Conclusion

Based on the FECM, integrated prediction of macroscopic properties of composites is realized by PCL in PATRAN. Because the processes of parameterized finite element modeling of RVE, establishing RVE library and integrating the calculated program of micromechanics have generality, that provide a new thought for composite structure design and analysis. At present, although there are few of RVE in RVE library and the solution type is only the linear elastic analysis, the good expansibility of RVE library and portability of calculation program lay a base to perfect and develop the system.

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