Composite Structures 122 (2015) 405–416

Contents lists available at ScienceDirect

Composite Structures

journal homepage: www.elsevier.com/locate/compstruct

Numerical homogenization for composite materials analysis. Comparison with other micro mechanical formulations

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ARTICLE INFO

Article history:
Available online 21 November 2014

Keywords:
Composites
Homogenization
Mechanical properties
Finite element method (FEM)

ABSTRACT

This work presents a two-scale homogenization procedure to analyze three dimension composite structures by FEM. The theory implemented is compared with other micro-structural formulations: micro models and serial–parallel mixing theory, in terms of result accuracy and computational cost. The comparison shows that for linear analysis, the homogenization is an excellent alternative to the other formulations. Its computational cost is substantially lower than the one required by the micro-model and it is able to capture several micro-structural phenomena that it is not automatically recorded by the serial–parallel methodology. It will also be shown that the extension of the proposed theory to the non-linear range stills represents a challenge. The major limitation is its computational cost because it requires to solve the sub scale at each gauss point and load step. However, the comparison shows that this cost is in terms of CPU time but not in terms of memory. Based on the results obtained, it can be concluded that the homogenization is an excellent alternative for simulation of materials with complex micro structures. The method is also very promising for non linear simulations, when coupled with a threshold criteria to decide whether it is necessary to analyze the RVE or not.

1. Introduction

The composites are non-homogeneous materials made of at least two different components. Generally, they are constituted by a matrix that embeds reinforcement elements [1]. These can be particles, short fibers, long fibers, etc. The different failure modes of a composite begin in its microstructure and then propagates, becoming larger and causing the final material failure. It is essential for a constitutive model to consider the microstructure if its objective is to predict the failure of the composite. Different methodologies have been proposed to obtain the behavior of the composite, taking into account its internal configuration. The most commonly used are: micro models, the mixing theory and the homogenization approaches.

A micro model is the simplest way to consider the microstructure of a composite because its internal structure is modeled explicitly. Currently these models are used to study local effects such as the contact, stress and strain produced by a steel ball sliding on the surface of a composite [2,3], to analyze of the propagation of a matrix crack from a debonded fiber [4], or to study the effect of the interface, for a particle reinforced metal matrix composite, in the macro tensile stress/strain curve [5], etc. The problem with this kind of models is that their use is limited by its computational cost.

The mixing theory was proposed initially by Truesdell and Toupin [6]. Later, Green and Adkins [7] presented a general non-lineal constitutive equation. Ortiz and Popov [8,9] proposed a constitutive equation for unreinforced concrete idealized as a composite material. Then, the theory was modified by Oller et al. [10] and Neamtu et al. [11] introducing the serial–parallel concept. The mechanical characteristic of the composite are obtained using the properties of each component and taking into account its topological distribution. Oller generalizes the mixing theory to enable the resolution of any composite with reinforced matrix, without the limitation required by the compatibility equation [12]. The SP continuum approach proposed by Rastellini et al. [13] assumes the behavior components of the composite as parallel materials in the fibers alignment direction and as serial materials in the orthogonal direction. Recently, Otero et al. [14] presented the extension of the mixing theory for the study of matrices reinforced with nanotubes.

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http://dx.doi.org/10.1016/j.compstruct.2014.11.041
0263-8223/

With the homogenization theory the problem is divided into two or more scales. One of the most relevant methods was proposed and developed by Sanchez-Palencia [15] and Bensoussan et al. [16], which is formulated in terms of asymptotic expansion theory. On the other hand, Suquet [17,18] uses the method of averages to solve and extend the problem in two scales to the non-linear case. Suquet laid the foundation of what today is known as first-order homogenization [19]. The deformation gradient tensor is used to solve the problem at the micro scale and then the macroscopic stress tensor is obtained using the averaging equation. Over time the method was extended to large deformations with arbitrary nonlinear material behavior at the micro scale, thanks to the work of Moulinec [20], Miehe [21–23], Terada [24,25]. Geers and Kouznetsova developed what is called second-order homogenization [26–28]; in this case the method uses the deformation gradient tensor and its Lagrangian gradient to solve a boundary value problem at the micro scale. The second-order approach allows solve the macro scale problem in the presence of moderate localization, as macroscopic deformation gradients (e.g. in bending) are passed to the RVE boundaries. To solve problems involving damage and fracture, leading to intense localization, a continuous-discontinuous homogenization has been developed [29]. It consists in the definition of a localization band at the macro scale, and using the deformation gradient tensor, in this band. In the last years, the homogenization has been extended to coupled thermo-mechanical problems [30], and to problems with cohesive zones [31], which can properly handle localization at the macroscopic scale.

This paper compares the results provided by these three numerical models (micro models, mixing and homogenization approaches), looking into the strengths and weaknesses of each one of them. In the next section a brief description of Micro models and the serial–parallel theory, is done. Sections 3 and 4 describe the homogenization framework proposed and its implementation for three dimension composite structures. In Section 5 it is described the numerical model used in Section 6 to compare the results obtained with the different theories. Section 7 presents a computational cost comparative study considering all theories. Finally, Section 8 contains the conclusion of this work.

2. Numerical models used to simulate the microstructural's behavior

This section briefly describes the numerical models that will be compared with the homogenization framework.

2.1. Micro models

In these models, the constituent materials forming the composite are modeled explicitly. Therefore, the response of the composite arises naturally. Each single material is modeled with its own constitutive law. These models are very powerful because they do not need to take any hypothesis on the microstructural behavior. However, their biggest limitation is its computational cost and in most cases their use is not practical.

2.2. Serial-parallel mixing theory

The serial–parallel mixing theory could be defined as a phenomenological homogenization, where the behavior of the composite is obtained from the constitutive response of their material components. This theory has been developed by Rastellini et al. [13], and is a natural evolution of the parallel mixing theory developed by Car et al. [32,33]. The theory is based on the compatibility conditions defined by Trusdell and Toupin [6], but introduces a modification in the iso-strain hypothesis. The iso-strain condition is imposed in the reinforcement direction (normally fiber) and a new iso-stress condition is imposed in the transversal directions. The theory is based on the following hypotheses:

1. The constituent materials of the composite are subjected to the same strain in the parallel (fiber) direction.
2. Constituent materials are subjected to the same stress in the serial direction.
3. The response of the composite material is directly related to the volume fractions of its constituent materials.
4. The phases in the composite are considered to be homogeneously distributed.
5. The constituent materials are considered to be perfectly bonded.

Taking only two composite components, the equations that define the stress (σ) equilibrium and setting up the strain (ε) compatibility between the individual components follow the hypothesis previously described are:

Parallel behavior:

$$\begin{aligned} {}^{c}\varepsilon_p &= {}^{m}\varepsilon_p = {}^{f}\varepsilon_p \\ {}^{c}\sigma_p &= {}^{m}k^{m}\sigma_p + {}^{f}k^{f}\sigma_p \end{aligned} \tag{1}$$

Serial behavior:

$$\begin{aligned} {}^{c}\varepsilon_s &= {}^{m}k^{m}\varepsilon_s + {}^{f}k^{f}\varepsilon_s \\ {}^{c}\sigma_s &= {}^{m}\sigma_s = {}^{f}\sigma_s \end{aligned} \tag{2}$$

where the superscripts c, m and f stand for composite, matrix and fiber, respectively and ${}^{i}k$ is the volume-fraction coefficient of each constituent in the composite.

This theory can predict the linear and non linear behavior of structural elements made of composite materials. Composite materials that can be modeled are those formed of long fibers embedded in a matrix. The theory predicts the different behavior of the composite, depending on the load direction. The potential of this theory is that it is capable to predict accurately the response of composites in the linear and non linear range (i.e. delamination failure) as has been proved in several papers [34,13,35–39,14,40]. On the other hand, The theory of serial–parallel mixtures is able to simulate the delamination problem naturally, without having to define specific elements or predefine the path of fracture.

3. Multi-scale homogenization model

The first-order homogenization framework presented here takes knowledge from the theory proposed by Zalamea [41] and later extended by Oller et al. [42] and by Badillo and Oller [43]. An extension to tri-dimensional framework of this theory is described in the following section.

The multi-scale homogenization is based on the use of an unit cell or representative volume element (RVE). The RVE definition corresponds to a microstructural subregion which is representative of the entire sub scale. The RVE is employed to determine the corresponding effective properties for the homogenized macro scale. For composites, it is assumed that it must contain a sufficient number of inclusions, which makes the effective moduli independent of assumed homogeneous forces or displacements on the RVE boundary.

In general, a multi-scale formulation that follows the first-order homogenization procedure can be identified as a "deformation driven" formulation. This mean that, with a deformation at the macro scale level, expressed by the strain tensor $\bar{E}$, the homogenized stress tensor $\bar{\sigma}$ and the homogenized constitutive tensor $\bar{C}$ can be determined at the sub scale level based on the interaction among the constituents at the RVE.