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Practical implementation of asymptotic expansion homogenisation in thermoelasticity using a commercial simulation software

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ABSTRACT

Asymptotic expansion homogenisation (AEH) is a rigorous homogenisation method that allows to model the thermomechanical behaviour of periodic materials in an efficient manner. The main advantages of this method are the reduction of the problem size and the capability of quantifying the strain and stress levels in the microscale using macroscale results. This method provides explicit equations for its purpose, an advantage not found on typical homogenisation methods.

This paper presents a pedagogic implementation and validation of AEH using the commercial simulation software ABAQUS. The scope of this work lies on thermoelasticity applied to heterogeneous materials. In this work, guidelines and troubleshooting for a successful implementation are analysed and discussed. Its purpose is to motivate the use of homogenisation methods, specially the AEH, and to detail every step needed to implement it using a commercial software. Key points, such as boundary conditions, computation of characteristic displacements and effective properties are discussed. Given the complexity of the problem, a series of validation schemes and results are presented and analysed. A user subroutine code is also presented.

1. Introduction

A large number of industrial and engineering materials are heterogeneous at a given level, consisting on different constituents that behave differently in some circumstances. Their behaviour can be dependent on many factors such as: (i) properties, (ii) spatial arrangements and (iii) volume fractions of constituents [1]. A direct approach can be done by spatially modelling each constituent of the heterogeneous material. Consequently, both properties and spatial distributions would be taken into account. However, this modelling approach often results in prohibiting computational costs. Therefore, the reduction of the referred costs without losing the proper characterisation of microstructure is needed [2]. This need can be fulfilled with homogenisation methods that replace the heterogeneous material with an equivalent homogeneous material. Asymptotic expansion homogenisation (AEH) allows to properly model the thermomechanical behaviour of heterogeneous materials, having two main tasks: dealing with a smaller material scale, called microscale, and simultaneously dealing with a larger structural scale, called macroscale. During this process, the macroscale is explicitly analysed using the information gathered on a detailed analysis of the microscale. The inverse approach can also be done. The detailing of the material behaviour in the microscale using the results of the macroscale is called localisation. Additionally, the asymptotic expansion homogenisation methodology allows the analysis of a great number of different microstructures, given the requirement of a periodic Representative Unit Cell (RUC) [3].

Nowadays, homogenisation is rapidly maturing due to the increasing power of computation. However, this subject dates back many years and started with homogenisation methods such as effective medium models of Eshelhy [4], Mori and Tanaka [5], Hashin–Shtrikman bounds [6], Halpin–Tsai equations [7], self-consistent approaches of Hill [8] and many others [1]. Afterwards, a new mathematical homogenisation method emerged as the asymptotic expansion homogenisation, pioneered by Bensoussan et al. in 1978 [9]. Then, many authors followed the subject, as Sanchez-Palencia in 1980 [10], Guedes and Kikuchi in 1990 [11], Hollister and Kikuchi 1992 [12], Terada and Kikuchi in 1996 [13], Chung et al. in 2001 [14], Yuan and Fish et al. in 2007 [15], Asada and Ohno et al. in 2007 [16], Pinho-da-Cruz et al. in 2007 [17], etc. Yuan and Fish in 2007 carried out an asymptotic expansion homogenisation implementation in the commercial

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computer-aided engineering software ABAQUS [15]. However, the homogenisation of the thermomechanical behaviour was not considered, the extension of the implementation to other problems raises several issues and the computational effort is not optimised. In the same year, Asada and Ohno proposed a different asymptotic expansion homogenisation approach based on an iterative methodology, where the computation was carried out based on an initial guess [16]. In this case, the implementation methodology could be extended to other problems, but the computation effort was dependent on the quality of initial guess. Commonly, these approaches lead to large computation times.

A two-dimensional model was developed using the commercial software ABAQUS, but the extension to a three-dimensional problem is straightforward. In the scope of this work, the two-dimensional case was chosen due to its simplicity, however the extension to a three-dimensional problem corresponds to tensorial adjustment in the formulation that can be consulted in [2].

The chosen model requires a programming task, but allows to control every step in the asymptotic expansion homogenisation process. Additionally, the paper details the implementation process including some pedagogic issues and specifications related to the implementation in a commercial software, as well as the troubleshooting of frequent problems. Therefore, it can be a good starting point for new researchers and students working in simulation modelling using homogenisation methods. In order to help the programming task, codes are provided as Appendixes. Moreover, the use of a commercial software allows a quickly implementation of the presented methodology, when compared to the development its own software.

In sum, none of previous authors have fully integrated a thermoelastic homogenisation methodology into a simulation commercial software. Furthermore, extensions of the present work are straightforward and the specific details of the model implementation might differ between different commercial software, the concepts and the guidelines on this paper remain valid.

This document starts with the introduction of the asymptotic expansion homogenisation methodology in its assumptions and differential formulation, allowing the analysis and discussion of the finite element approximation of the variational problem and its implementation. In the end some results, validation schemes and conclusions are presented.

2. Homogenisation in thermoelasticity: mathematical formulation

The formulation presented in this section is based on references [2,14,17,18]. The asymptotic expansion homogenisation is a homogenisation method capable of modelling the thermomechanical behaviour of periodic materials in an uncoupled and quasi-static process. The main advantages of this method are: (i) the capability of reducing the number of degrees of freedom linked to modelling the thermomechanical behaviour and (ii) allowing the proper characterisation of periodic microstructures [17].

Consider a linear thermoelastic heterogeneous material associated to a material body Ω. The microstructure of Ω is formed by a periodic repetition of a representative unit-cell associated to the region Y [19]. The relation ϵ of the dimensions of the microstructure and the macrostructure is very small ($\epsilon \ll 1$) for the majority of the heterogeneous materials with periodic structure. The thermomechanical loading of such materials creates periodic oscillations on the resulting displacements, stress or strains, being these oscillations the consequence of the periodic arrangement of constituents of the material. At this point, it's common to assume two distinct scales: $\boldsymbol{x}$ and $\boldsymbol{y}$ for the behaviour of the materials in the macroscale and in the microscale, respectively [13,17]. Thus, the variables related to the referred fields become functionally dependent on both $\boldsymbol{x}$ and $\boldsymbol{y}$ scales, where

$$\boldsymbol{y} = \boldsymbol{x}/\epsilon. \tag{1}$$

The referred functional dependence is usually called Y-periodicity. The Y-periodicity of the microstructural heterogeneities reflects itself on the fact that the thermal expansion tensor $\boldsymbol{\alpha}$ and the elasticity tensor $\mathbf{D}$ are Y-periodic in $\boldsymbol{y}$. In contrast, the material homogeneity at the macroscale level results from the fact that these tensors do not depend on the macroscale system of coordinates $\boldsymbol{x}$, resulting

$$\alpha_{ij} = \alpha_{ij}(\boldsymbol{y}) \quad \text{and} \tag{2}$$

$$D_{ijkl} = D_{ijkl}(\boldsymbol{y}). \tag{3}$$

On the macroscale $\boldsymbol{x}$, the microscale constituents appear over periods ϵ^{-1} times smaller than the characteristic dimension of $\boldsymbol{y}$. Using Eq. (1), Eqs. (2) and (3) result in

$$\alpha^{\epsilon}_{ij} = \alpha_{ij}(\boldsymbol{x}/\epsilon) \quad \text{and} \tag{4}$$

$$D^{\epsilon}_{ijkl} = D_{ijkl}(\boldsymbol{x}/\epsilon), \tag{5}$$

respectively, where the superscript ϵ states that $\boldsymbol{\alpha}$ and $\boldsymbol{D}$ are ϵY-periodic in the macroscale, $\boldsymbol{x}$.

Assuming infinitesimal strains and a quasi-static process, the linear thermoelastic problem is given by the following equations:

$$\frac{\partial \sigma^{\epsilon}_{ij}}{\partial x^{\epsilon}_j} + f_i = 0 \text{ in } \Omega, \tag{6}$$

$$\varepsilon^{\epsilon}_{ij} = \frac{1}{2}\left(\frac{\partial u^{\epsilon}_i}{\partial x^{\epsilon}_j} + \frac{\partial u^{\epsilon}_j}{\partial x^{\epsilon}_i}\right) \text{ in } \Omega \text{ and} \tag{7}$$

$$\sigma^{\epsilon}_{ij} = D^{\epsilon}_{ijkl}\varepsilon^{\epsilon}_{kl} - \beta^{\epsilon}_{ij}\Delta T^{\epsilon}, \tag{8}$$

where

$$\Delta T^{\epsilon} = T^{\epsilon} - T_0, \tag{9}$$

$$\beta^{\epsilon}_{ij} = \beta^{\epsilon}_{ij}(\boldsymbol{x}/\epsilon) \quad \text{and} \tag{10}$$

$$\beta^{\epsilon}_{ij} = D^{\epsilon}_{ijkl}\alpha^{\epsilon}_{kl}. \tag{11}$$

σ^{ϵ}_{ij} and $\varepsilon^{\epsilon}_{ij}$ are the components of the Cauchy stress and strain tensors, respectively. f_i, u_i and T_0 are the loads per unit of volume, displacements and reference temperature, respectively. On the boundary Γ of Ω, the Dirichlet (Γ_{D}) and Neumann (Γ_{N}) boundary conditions can be established as

$$u^{\epsilon}_i = \bar{u}_i \quad \text{in} \quad \Gamma_{\mathrm{D}} \quad \text{and} \tag{12}$$

$$\sigma^{\epsilon}_{ij}n_j = \bar{t}_i \quad \text{in} \quad \Gamma_{\mathrm{N}}, \tag{13}$$

where $\Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{N}} = \Gamma$ and $\Gamma_{\mathrm{D}} \cap \Gamma_{\mathrm{N}} = \emptyset$. $\bar{u}_i$ and $\bar{t}_i$ are the prescribed values of displacements and surface load values, respectively. n_j are the components of an outward vector normal to the surface Γ_{N}.

Considering the existence of two distinct scales, which connect the material behaviour of the macroscale Ω and the microscale Y, the displacement fields can be approximated by an asymptotic expansion in ϵ, mathematically given by

$$u^{\epsilon}_i = u^{(0)}_i(x,y) + \epsilon u^{(1)}_i(x,y) + \epsilon^2 u^{(2)}_i(x,y) + \cdots, \tag{14}$$

where $u^{(r)}_i(x,y)$, with $r \in \mathbb{N}_0$ and $i \in \{1,2,3\}$, are Y-periodic functions in $\boldsymbol{y}$, called correctors of order r of the displacement field.