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# On the characterisation of elastic properties of long fibre composites using computational homogenisation ☆

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ABSTRACT

This paper addresses the prediction of the elastic properties of long fibre-reinforced composites from the finite element-based computational homogenisation of a Representative Volume Element (RVE) in the range of moderately large strains. The macroscopic elastic properties are estimated by matching the reference tangential elasticity tensors of the homogenisation-based model and an assumed transversely isotropic hyperelasticity model. The effectiveness of the approach is illustrated by means of a numerical example where the solution of a boundary value problem obtained with the assumed hyperelastic model and the predicted parameters is compared with that obtained with a fully coupled multi-scale simulation.


## 1. Introduction and background

Accurate micro-mechanically-based predictions of elastic constants of a composite, which take the shape, size and distribution of the reinforcement into account, as well as the material properties of both the matrix and the reinforcement are very desirable in engineering design, as they offer the possibility of tailoring the composite for specific needs. The use of homogenisation methods based on the volume averaging of the strain and stress field over a *Representative Volume Element* (RVE) to tackle this problem has been reported in the literature since the 1980s. In this context, Adams and Crane [1] used distinct kinematical constraints over the RVE boundary for normal and shear loading, while Zhang and Evans [38] and Shi et al. [29] used axisymmetric unit cells. Brockenbrough et al. [4] investigated fibre packing and shape on the overall properties using linear RVE boundary kinematical constraints, while more recently Grasset-Bourdel et al. [11] proposed a technique for optimisation of 3D RVE for anisotropy index reduction in modelling thermoelastic properties of two-phase composites using a periodic homogenisation method. Sun and Vaidya [34] imposed separate RVE boundary conditions for each property sought, Xia et al. [37] extracted the material properties of a square packed periodic RVE from the compliance matrix. Michel et al. [21] proposed a methodology based on a Fast Fourier Transform as an alternative for the more conventional finite element-based analysis.

A number of publications have appeared in the literature using homogenisation for predicting mechanical behaviour of long fibre composites in the small strain regime. Theocaris et al. used 2-D RVE's to study fibre reinforced composites with linear elastic constituents [36] and compared with existing analytical solutions. Also limited to small strain regime, Dong et al. compared fibre packing arrangements using embedded unit cells [8], but incorporated a non-linear strain-hardening matrix. Macroscopic non-linear parameter estimation under finite straining is a rather less researched area. Notable publications include [13], where Guo et al. estimated the strain energy function for the composite by using generalised Halpin-Tsai equations, as well as Lahellec et al. [18] and Brun et al. [5], who obtained estimates of the macroscopic behaviour of hyperelastic composites using the second-order method of Castañeda [6] and Castañeda and Tiberio [7].

We propose a methodology to estimate the parameters of an assumed transversely isotropic hyperelastic constitutive model in the range of moderately large strains, based on matching its reference tangential elasticity tensor with that of the computational homogenisation-based multi-scale model. The effectiveness of the procedure is illustrated by means of a numerical example where the finite element solution of a boundary value problem obtained with the assumed hyperelasticity model and the predicted parameters is compared with that obtained with a fully coupled multi-scale simulation.

The layout of the paper is as follows: First, a brief introduction to a general large strain multi-scale constitutive theory and its implementation in the finite element setting is presented in Section 2. The proposed procedure for the parameter identification

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methodology to the range of moderately large strains is presented in Section 3 together with the numerical example used in its verification. Some concluding remarks are made in Section 4.

## 2. Multi-scale constitutive modelling at large strains

The class of homogenisation-based multi-scale constitutive models employed in the present study is characterised by the assumption that the strain and stress tensors at a point of the so-called *macro-continuum* (see Fig. 1) are volume averages of their respective microscopic counterpart fields over a pre-specified *Representative Volume Element* (RVE) [9,16,17]. That is, by defining the *deformation gradient* $\bar{\boldsymbol{F}}$ and the *first Piola–Kirchhoff stress tensor* $\bar{\boldsymbol{P}}$ as volume averages of their counterpart fields over the RVE [22], we have

$$\bar{\boldsymbol{F}} \equiv \frac{1}{V}\int_{\Omega} \boldsymbol{F}\, dV = \frac{1}{V}\int_{\Omega} (\boldsymbol{I} + \nabla \boldsymbol{u})\, dV, \tag{1}$$

and

$$\bar{\boldsymbol{P}} \equiv \frac{1}{V}\int_{\Omega} \boldsymbol{P}\, dV, \tag{2}$$

where $\boldsymbol{F}$ and $\boldsymbol{P}$ denote, respectively, the deformation gradient and first Piola–Kirchhoff stress fields of the RVE, $V$ is the volume of the RVE and $\nabla$ denotes the gradient operator.

Here we focus on RVEs with constituents modelled by hyperelasticity. Hence, $\boldsymbol{P}$ and $\boldsymbol{F}$ are related by the general hyperelasticity potential law

$$\boldsymbol{P}(\boldsymbol{x}) = \frac{\partial \psi_{\boldsymbol{x}}}{\partial \boldsymbol{F}(\boldsymbol{x})}, \tag{3}$$

where $\psi_{\boldsymbol{x}}$ denotes the given free-energy function of point $\boldsymbol{x}$ of the RVE with respect to its argument $\boldsymbol{F}$.

By defining the field $\tilde{\boldsymbol{u}}$ of *displacement fluctuations* of the RVE as

$$\tilde{\boldsymbol{u}} \equiv \boldsymbol{u} - \boldsymbol{u}^*, \tag{4}$$

with

$$\boldsymbol{u}^*(\boldsymbol{x}) \equiv (\bar{\boldsymbol{F}} - \boldsymbol{I})\boldsymbol{x}, \quad \forall \boldsymbol{x} \in \Omega, \tag{5}$$

the deformation gradient field of the RVE can be written as a sum

$$\boldsymbol{F}(\boldsymbol{x}) = \bar{\boldsymbol{F}} + \widetilde{\boldsymbol{F}}(\boldsymbol{x}), \tag{6}$$

of a uniform deformation gradient coinciding with the macroscopic deformation gradient and a displacement fluctuation gradient field,

$$\widetilde{\boldsymbol{F}} \equiv \nabla \tilde{\boldsymbol{u}}. \tag{7}$$

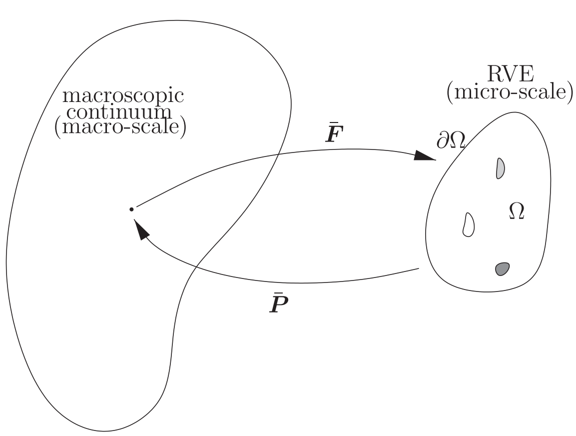


**Fig. 1.** Multi-scale model. The macro-continuum and the RVE.

The RVE equilibrium problem in the present case consists of finding, for a given macroscopic deformation gradient $\bar{\boldsymbol{F}}$, a kinematically admissible displacement fluctuation field $\tilde{\boldsymbol{u}} \in \mathscr{V}$, such that

$$\int_{\Omega} \boldsymbol{P}(\bar{\boldsymbol{F}} + \nabla \tilde{\boldsymbol{u}}) : \nabla \boldsymbol{\eta}\, dV = 0 \quad \forall \boldsymbol{\eta} \in \mathscr{V}, \tag{8}$$

where $\mathscr{V}$ is the (as yet not defined) space of virtual kinematically admissible displacements of the RVE.

### 2.1. Linearised equilibrium and homogenised first elasticity tensor

Crucial to the finite element solution of the non-linear equilibrium problem at the heart of the homogenisation-based multi-scale model is the linearisation of the equilibrium Eq. (8). The linearisation of (8) at a configuration of the RVE defined by an arbitrary deformation gradient field $\boldsymbol{F} = \boldsymbol{F}^*$ consists of finding $\delta\tilde{\boldsymbol{u}} \in \mathscr{V}$, such that

$$\int_{\Omega} \boldsymbol{A} : \nabla \delta\tilde{\boldsymbol{u}} : \nabla \boldsymbol{\eta}\, dV = -\int_{\Omega} \boldsymbol{P} : \nabla \boldsymbol{\eta}\, dV \quad \forall\, \boldsymbol{\eta} \in \mathscr{V}, \tag{9}$$

where

$$\boldsymbol{A}(\boldsymbol{x}) = \left.\frac{\partial \boldsymbol{P}(\boldsymbol{F})}{\partial \boldsymbol{F}}\right|_{\boldsymbol{F}=\boldsymbol{F}^*(\boldsymbol{x})}, \tag{10}$$

is the microscopic *first elasticity tensor* field and

$$\boldsymbol{P}(\boldsymbol{x}) = \frac{\partial \psi_{\boldsymbol{x}}}{\partial \boldsymbol{F}^*(\boldsymbol{x})}. \tag{11}$$

In the present case, it is possible to derive a closed form for the *homogenised first elasticity tensor*, i.e. the fourth-order tensor that expresses the tangential relationship between macroscopic first Piola–Kirchhoff stress and the macroscopic deformation gradient:

$$\bar{\boldsymbol{A}} \equiv \frac{\partial \bar{\boldsymbol{P}}}{\partial \bar{\boldsymbol{F}}}. \tag{12}$$

It can be shown [21,32] that the homogenised first elasticity tensor has the representation

$$\bar{\boldsymbol{A}} = \boldsymbol{A}^{\text{avg}} + \widetilde{\boldsymbol{A}}, \tag{13}$$

where $\boldsymbol{A}^{\text{avg}}$ is the volume average of the microscopic first elasticity tensor:

$$\boldsymbol{A}^{\text{avg}} = \frac{1}{V}\int_{\Omega} \boldsymbol{A}\, dV, \tag{14}$$

and $\widetilde{\boldsymbol{A}}$ is defined by the Cartesian components

$$\widetilde{A}_{ijkl} = \frac{1}{V}\int_{\Omega} A_{ijpq}[\nabla \tilde{\boldsymbol{u}}_{kl}]_{pq}\, dV, \tag{15}$$

with $\tilde{\boldsymbol{u}}_{kl} \in \mathscr{V}$, being the solutions to the linear variational equations

$$\int_{\Omega} \nabla \boldsymbol{\eta} : \boldsymbol{A} : \nabla \tilde{\boldsymbol{u}}_{kl}\, dV = \left[-\int_{\Omega} \nabla \eta : \boldsymbol{A}\, dV\right] : \boldsymbol{e}_k \otimes \boldsymbol{e}_l \quad \forall \boldsymbol{\eta} \in \mathscr{V}. \tag{16}$$

### 2.2. RVE kinematical constraints

Different choices of space $\mathscr{V}$ will in general result in different estimates $\bar{\boldsymbol{A}}$ for the macroscopic elasticity tensor. This is clear from (15) and (16) as the components of $\widetilde{\boldsymbol{A}}$ depend on the fields $\tilde{\boldsymbol{u}}_{kl}$ which, in turn, are generally dependent upon the choice of $\mathscr{V}$ (see [32] for further details on variational basis and [26,23] for finite element implementation in the small strain context). The space $\mathscr{V}$ of virtual kinematically admissible displacements defines the kinematical constraints enforced upon the RVE. The commonly used constraints are the following: