Multiscale homogenization model for wood and the variables influence over the mechanical properties

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Abstract. Wood has great potential as a structural material with excellent strength, lightweight, thermal insulation, and acoustical properties. However, its hierarchical nature and complexity represent a challenge in wood structure's design and manufacture. Homogenization can be a helpful tool for understanding wood behavior, encouraging wood usage as a structural material for new applications. The homogenization method calculates the effective properties of a material with many heterogeneities, represented as a base cell that repeats itself over the continuum. This base cell is called Representative Element volume (RVE), a volume with all the information necessary to describe the geometry of the different phases and the local material properties. This work uses a displacement-based approach with Finite Element Method (FEM) to calculate six boundary conditions applied over the RVE, where each boundary condition relates to a different stiffness matrix component. The result is a homogenized material at the macroscale, considering the mechanical properties of each phase and its distribution over the RVE. This work identifies the most important variables for each scale and discusses its influence over the effective properties. The homogenization method allows for a better understanding of the different variables that influence the mechanical properties of wood at each scale.

Keywords: Computational homogenization, Multiscale, Wood structure, Cellular material, Finite element method

1 Introduction

Wood is a natural material sustainable for the environment, representing a significant advantage for the construction industry nowadays. Its use as a structural material has increased given the necessity for reducing carbon footprints, increasing energy and water security concerns, and the desire for sustainable industrial growth [1]. Despite these benefits, there are certain disadvantages associated with natural materials usage. These materials are usually expensive due to their limited availability, and their supply and quality can vary with climatic conditions [2]. Additionally, its mechanical properties can significantly vary across wood species and with variables such as moisture, density, and microstructure. Understanding wood's hierarchical nature can open alternatives to create new cellular materials that can supply that demand or even increase wood performance in the future.

Micromechanical models for wood deformation and strength are classified into three groups: cellular models, continuum micromechanics, and homogenization-based methods, which consider wood as a composite [3]. Several works have considered only the micro-scale, such as Naik and Fronk [4], which used a finite element model to determine the cell wall properties and the cellulose volume fraction influence. Qing and Mishnaevsky [5] also employed multiscale homogenization to model the moisture transport in wood and the moisture content effect over the cell wall elastic properties.

The relationship between the cell wall geometry and mechanical properties was considered by Sjölund et al. [6], showing the effect of the cell shape and cell wall properties on the wood's effective rigidity. Qing and Mishnaevsky [7] extended the same analysis for the meso scale. Recently the computational approach has gained popularity by expanding the analysis to every scale. Saavedra Flores et al. [8]-[9] and Rojas Vega et al. [10] considered this approach to determine the mechanical and thermomechanical properties of timber. In this work, the homogenization method is also applied sequentially to determine the final properties at the macro-scale.

2 Homogenization Method Implementation

The homogenization theory is an alternative approach to finding the effective properties of a material with a large number of heterogeneities. This approach reduces the problem complexity by replacing the heterogeneous material with a homogenous one, with the homogenized property. Homogenization theory has applications in physics and engineering with multiple approaches available. The formulation considered in this work uses the RVE (Representative Volume Element) approach with appropriate boundary conditions to find the equivalent elastic tensor for the homogenous material, as explained in the work of J.Yvonnet [11]. An RVE is a volume where the geometry of the different phases and the local material properties are assumed to be known.

First it is consider that given a macroscopic strain ε is necessary to find a displacement field $\boldsymbol{u}(\boldsymbol{x})$ in the domain Ω such that:

$$\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x})) = 0 \quad \forall \boldsymbol{x} \in \Omega, \tag{1}$$

with

$$\boldsymbol{\sigma}(\boldsymbol{u}(\boldsymbol{x})) = \boldsymbol{C}(\boldsymbol{x}) : \varepsilon(\boldsymbol{u}(\boldsymbol{x})), \tag{2}$$

$$\varepsilon(\boldsymbol{u}(\boldsymbol{x})) = \frac{1}{2}(\nabla \boldsymbol{u}(\boldsymbol{x}) + \nabla^T \boldsymbol{u}(\boldsymbol{x})) \tag{3}$$

and verifying

$$\bar{\varepsilon} = \int_{\Omega} \varepsilon d\Omega. \tag{4}$$

Where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\boldsymbol{C}$ is the elasticity tensor. Equations (1) and 2 represent the equilibrium equation's strong form and the stress-strain relationship respectively. Equation 3 is the linearized strain tensor and eq.(4) states that the macroscopic strain applied over the RVE $\bar{\varepsilon}$, must be equal to the strain volume average over the domain.

According to J.Yvonnet [11], two boundary conditions satisfy eq.(4): kinematically uniform boundary condition (KUBC) and periodic boundary conditions (PER). For our case, periodic boundary conditions were chosen as the better alternative, and the displacement field $\boldsymbol{u}(\boldsymbol{x})$ takes the form:

$$\boldsymbol{u}(\boldsymbol{x}) = \bar{\varepsilon}\boldsymbol{x} + \widetilde{\boldsymbol{u}}(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Omega, \tag{5}$$

Where $\widetilde{\boldsymbol{u}}$ is a fluctuating displacement that is periodic on Ω. These periodic boundary conditions are imposed by constraining the node displacement of two nodes a and b on opposite faces of the RVE using eq. (5), such as:

$$\begin{aligned} u_i(\boldsymbol{x}^a) &= \bar{\varepsilon}_{ij} x_j^a + \widetilde{u}_i(\boldsymbol{x}^a) \\ u_i(\boldsymbol{x}^b) &= \bar{\varepsilon}_{ij} x_j^b + \widetilde{u}_i(\boldsymbol{x}^b) \end{aligned} \tag{6}$$

Given that the fluctuation is periodic $u_i(\boldsymbol{x}^a) = u_i(\boldsymbol{x}^b)$ and using eq. (6), it is possible to establish the boundary conditions for the contour nodes as follows:

$$u_i(\boldsymbol{x}^a) - u_i(\boldsymbol{x}^b) = \bar{\varepsilon}_{ij}(x_j^a - x_j^b) \tag{7}$$

Once the appropriate boundary conditions are established, the tensor $\boldsymbol{C}$ can be calculated. According to Barbero [12], the relationship between average stress and strain in the homogeneous composite material can be written as:

$$\bar{\sigma}_{ij} = C_{ijkl}\bar{\varepsilon}_{ij} \tag{8}$$

By choosing a unit value for the applied strain and considering the periodic conditions established in eq. (8), it is possible to compute the elastic matrix column by column:

$$C_{ijkl} = \bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij}(x_1, x_2, x_3) \quad \text{with} \quad \bar{\varepsilon}_{ij} = 1 \tag{9}$$

Wood is an orthotropic material, so six elastic models are necessary to compute all the values in $\boldsymbol{C}$ for the 3D case, corresponding to the six possible strains that could be applied over the RVE: $\bar{\varepsilon}_{11}$, $\bar{\varepsilon}_{22}$, $\bar{\varepsilon}_{33}$, $\bar{\varepsilon}_{12}$, $\bar{\varepsilon}_{13}$ and $\bar{\varepsilon}_{23}$. When a strain condition is imposed, the strains in the other directions must be zero.

The algorithm for imposing the periodic boundary conditions over the RVE is taken from Barbero [12] and adapted to Python using the interactive mode Pyansys [13] for each FEM analysis. The integral in eq. (9) can also be calculated using Pyansys to obtain the RVE average stress. The homogenization implementation considers three main stages: the RVE modeling according to each phase distribution and its mechanical properties. With this data, the periodic boundary conditions are applied on opposite faces of the RVE for each load case. Once the six FEM analyses are completed, it is possible to compute the matrix $\boldsymbol{C}$. The homogenized material properties can be easily calculated with the elastic tensor.

3 Multiscale Wood Homogenization

Wood species are classified into two main groups: softwoods, or coniferous trees, such as pine, cedar, and spruce, and hardwoods, such as balsa, beech, maple, and oak. The mechanical properties between categories can vary considerably, given fundamental differences in density and microstructural arrangements.

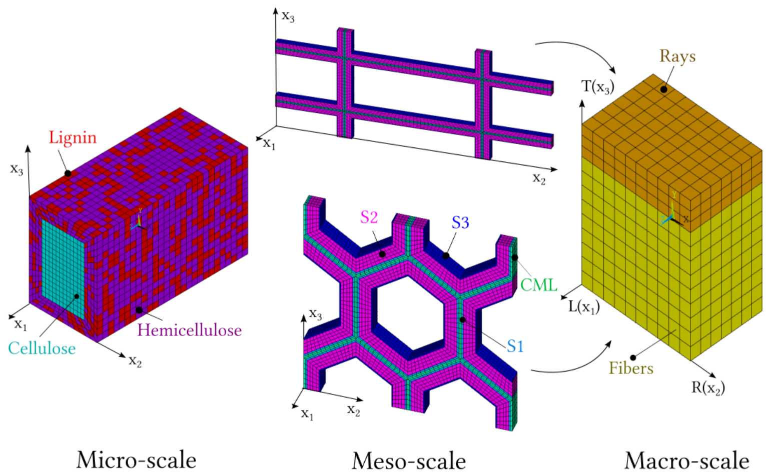

Figure 1. Discretized Representative Volumes for the micro, macro, and meso scales.

Many works in the literature examine softwood structures at different scales and their influence on their mechanical properties. To extend the analysis for hardwoods, Malek and Gibson [14] work is considered here as a reference for the RVE geometry and mechanical properties. The model was simplified from five scales to only three to reduce the analysis's complexity. Figure 1 shows the different phases and their distribution on each scale.

The microscale involves three materials: cellulose, hemicellulose, and lignin, with the mechanical properties presented in Table 1. The RVE has a cellulose core covered with a matrix of lignin and hemicellulose randomly arranged. At the micro-scale, the RVE has a rectangular cross-section of 9 nm x 12 nm and a length of 20 nm. These three components in the microfibril vary their proportions according to the cell wall material under consideration, as seen in Table 2. The wood cell wall is modeled as a symmetric seven-layer composite with one compound middle layer (CML) and six secondary walls (S1, S2, and S3) [14]. Therefore, the output data for the first homogenization step results in the mechanical properties of these four cell wall layer materials. The microfibrils in each layer also have an orientation concerning the longitudinal axes called the microfibril angle (MFA). Microfibril angles considered for every cell wall material at the meso-scale can be seen in Table 2.

Table 1. Elastic constants of cellulose, lignin and hemicellulose used in the micro-scale [14]

Material	E_1	E_2	E_3	G_{12}	G_{13}	G_{23}	v_{12}	v_{13}	v_{23}
Cellulose	111 GPa	24.6 GPa	7.51 GPa	3.43 GPa	6.85 GPa	3.23 GPa	0.11	0.15	0.40
Hemicellulose	9 GPa	4.5 GPa	4.5 GPa	2.25 GPa	2.25 GPa	1.67 GPa	0.35	0.35	0.35
Lignin		5.68 GPa			2.06 GPa			0.38	

The second homogenization step includes two different RVEs: fibers and rays. Figure 1 illustrates this, showing fibers and rays represented by a hexagonal and rectangular shape, respectively. The cell wall thickness for individual layers CM, S1, S2, and S3 is adjusted depending on the volumes assigned in Table 2. Finally, the last homogenization step is at the macro scale with a unit cell composed of rays and fibers. The RVE is a rectangular prism with a width=382 μm, height=320.8 μm, and length=251 μm.

Table 2. Cell wall composition data used as input on the meso-scale [14]

Layer	Volume	Cellulose	Hemicellulose	Lignin	MFA
S1	8 %	45%	35%	20%	70°
S2	72.67 %	50%	27%	23%	1.4°
S3	10.67 %	35 %	30 %	35 %	-70°
CML/2	8.66	3%	35%	62%	random

To validate the homogenization procedure, the results for each stage were compared with the results reported by Malek and Gibson [14], finding good coincidences with the expected results and obtaining an error of less than 15 % for the Young Modulus E_L overall. At each length scale, the constituents were assumed to be perfectly bonded and to remain linear elastic during loading.

4 Sensitivity Analysis

The hierarchical model proposed for hardwoods can be used to evaluate the Young Modulus E_L variability, with different parameters at every scale. At the microscale, the chosen variables are the volume fraction of cellulose f_c and hemicellulose f_h. The lignin percentage is adjusted accordingly to obtain the properties of layer S2. The S2 layer has a relevant effect on the cell wall stiffness, being the thickest layer within the wall, with almost 80% volume [2]. Therefore, only variations in S2 will be studied as seen in previous works [9]. The remaining layers CML, S1, and S2 will be unaltered. Figure 2b illustrates the RVE at the micro-scale with different volume fractions of lignin, hemicellulose, and cellulose. The code adapts to the input variables f_c and f_h, appropriately changing the material distribution. For this analysis at the micro-scale, the parameters of the subsequent homogenization steps remain constant.

The most important parameters at the meso-scale are the thickness t, the microfibril angle MFA, and fiber and ray cells dimensions denoted by h and l (see Fig. 2a). However, in the rectangular RVE associated with wood rays, h, and l are fixed at 18 μm, given that rays don't show significant variations in geometry with overall

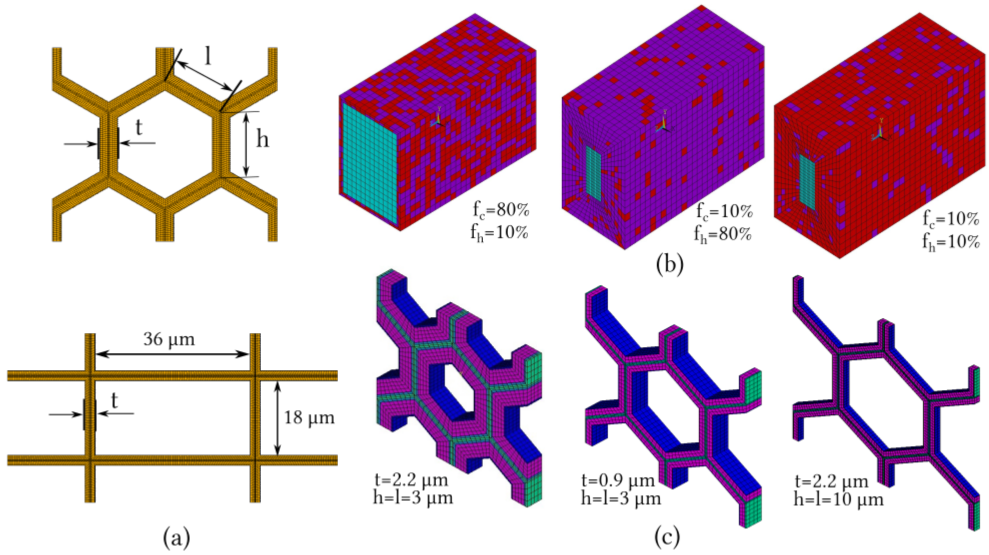

Figure 2. RVE variations for the sensitivity analysis. (a) Geometrical parameters at the meso-scale. (b) RVEs with different values of f_c and f_h. (c) RVEs with different t and h combinations

density. Consequently, t and MFA are the only variables considered for the ray's RVE. For fibers, the influence of parameters h and l is explored, with a variation range between 3 μm and 30 μm, as observed by Malek and Gibson [14]. The microfibril angle will vary between 0° and 20° and the thickness between 0.3 μm and 2.2 μm, as suggested in Shishkina et al. [2] work. Figure 2 illustrates the variations in the hexagonal RVE with the chosen parameters. By increasing the cell wall thickness and reducing h and l, more dense structures appeared, considering cell repetition over the continuum. Finally, the only variable available at the macro scale is the fiber volume fraction f_f.

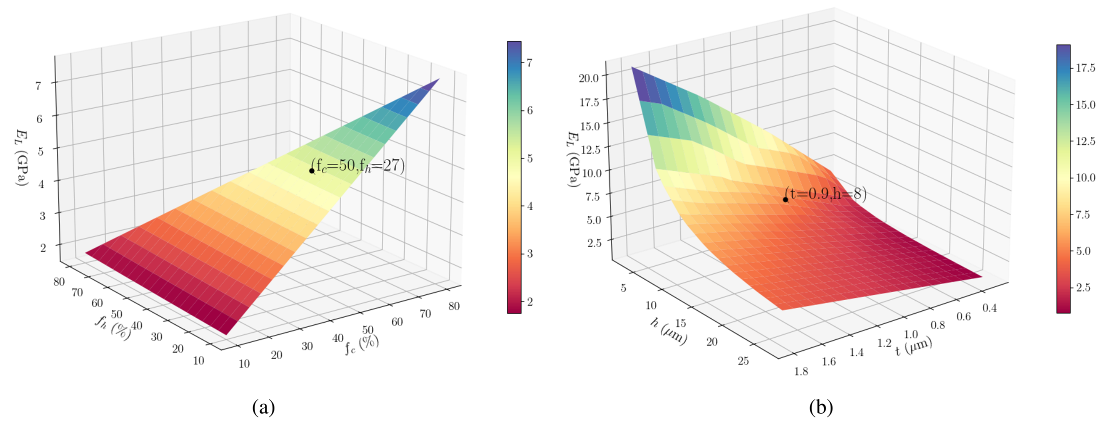

Figure 3. Longitudinal Young's modulus variation with parameters: (a) f_c and f_h. (b) h and t.

The micro-scale variable's influence on the longitudinal Young Modulus E_L is depicted in Fig.3a. In this case, the volume fractions f_c and f_h vary between 10 and 80% even though the variables at the meso and macro scale remain constant (MFA = 1.4°, t = 0.9μm, h = l = 8μm, f_f = 80%). Under these conditions, E_L varies between 1.57 and 7.51 GPa. In addition, f_c determines the increase in E_L, while f_h is not a decisive factor. Hence, an increase in the cellulose volume fraction in the microfiber RVE can increase the wood's mechanical properties on the macroscale. The point in Fig. 2a represents the values f_c and f_h commonly used for the S2 layer in balsa. A minor increase in properties is noticeable for higher values of f_h, but this effect is minimal compared to the gain associated with cellulose augmentation.

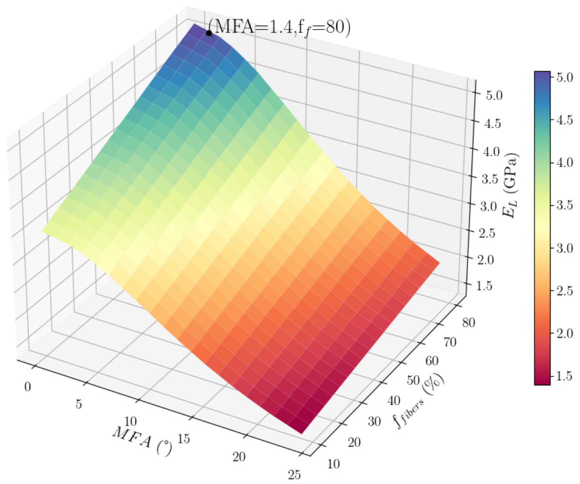

Figure 4. Longitudinal Young's modulus variation with parameters MFA and f_f at the macro scale.

Figure 3b shows the result for variations in the meso-scale, specifically the parameters h and t. The hexagonal cell geometry related to fibers is often regular, so h=l was considered for all cases. Again, the reference values for h and t represent one point on top of the surface. The Young modulus E_L varies non-linearly with the parameter h and decreases as h becomes larger. In terms of thickness, the relationship is linear, and the property increases with high values for t. The longitudinal Young modulus can vary between 0.678 and 20.98 GPa for the two variables examined. Malek and Gibson [14] work presented this behavior at the meso-scale level.

Finally, the microfiber angle influence and the fiber volume fraction at the macroscale are evaluated and shown in Fig. 4. The relationship between MFA and Young's modulus E_L is also non-linear, decreasing in value as the MFA angle increases. Moreover, raising the fibers' volume fraction results in higher values for E_L, a behavior already observed in Shishkina et al. [2] models. However, this increase is lower than the gains associated with MFA reduction. Young's modulus E_L fluctuates between 1.4 and 5.14 GPa for all the combinations considered, while other variables remain constant (t = 0.9 μm, h = l = 8 μm, fc = 50 %, fh = 27%). These results showed that the microfibril angle MFA and the parameters related to wood density, h, l, and t, have a higher influence over the longitudinal Young modulus, a behavior already explored by Lloyd [15].

5 Conclusions

The homogenization method represents a great alternative to predict the wood's mechanical properties at every scale according to its specific characteristics. The multiscale model proposed for hardwoods involved three homogenization steps in which input parameters vary across all scales. The algorithm reshapes the RVE geometry according to the input values required to obtain the new mechanical properties.

The most relevant parameters for wood's high longitudinal Young's modulus at the macroscale are the microfiber angle MFA and the variables t, h, and l related to the fiber's hexagonal configuration. The cellulose fraction at the microscale is also crucial to increasing the mechanical properties studied, given that highly influences the layer's stiffness at the mesoscale. Analyzing the different variables' influence on wood mechanical properties at the macro-scale allows the exploration of new materials inspired by wood that can potentially meet its high demand. Additionally, it can help improve the characteristics of existing wood species by favoring the desirable parameters already identified.

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