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Modeling Random Fiber Networks in Hyperelastic Composites

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Abstract. The mechanical behavior of elastomers reinforced with random fiber networks (RFNs) depends strongly on the microstructural organization. This work presents a computational approach for generating three-dimensional RFNs using a persistent random walk with orientation via the von Mises-Fisher distribution. The algorithm incorporates curvature control, fiber smoothing, and a self-avoidance criterion with collision detection to avoid fiber overlap. Fiber geometries are generated according to a target volume fraction through an iterative adjustment of the number of fibers and are exported for finite element analysis. The geometries of polyester fiber modeled as linear-elastic REINF264 elements in ANSYS are embedded into a hyperelastic RTV silicone rubber matrix modeled by a two-term Mooney-Rivlin formulation. Fibers were modeled as linear elastic reinforcement elements using REINF264 elements. Seven RVE sizes from 1 mm to 4 mm were tested under uniaxial deformation, and homogenized Cauchy stresses were computed to obtain the second Piola-Kirchhoff stress tensor and the effective material elasticity component $\mathbb{C}_{1111}$. Results indicate convergence of the elastic response for $L = 3.5\text{mm}$, suggesting this as the minimum RVE size for representing the given microstructure.

Keywords: random fiber networks, nonlinear materials, finite element analysis, microstructural modeling.

1 Introduction

Composite materials are widely used in weight-sensitive fields, such as aerospace and spacecraft, offering high strength and stiffness ratios essential for advanced lightweight structures [1]. Among the various types of reinforcement, random fiber networks (RFNs) stand out because of their complex and disordered fiber arrangement. Their unique properties, such as high porosity, flexibility, and large specific surface area, are directly linked to the complexity of their microstructural organization [2]. Accurately modeling these microstructures remains a challenge due to their inherent randomness and variability, affecting the overall mechanical response of the composite. Traditional modeling often offers oversimplified representations, limiting the assertiveness of the generated results.

Continuum mechanics assumes that distribution of material, stress, and strain within the infinitesimal neighborhood of a typical macroscopic particle (macro-element) is uniform. However, at the microscale, the neighborhood is generally heterogeneous due to the presence of distinct material phases or structural features.

The Representative Volume Element (RVE) is defined as the smallest volume of microstructure capable of accurately representing a given macroscopic property. Analyzing the RVE involves solving a boundary value problem and establishing a relationship between the averaged microscopic variables and their macroscopic counterparts. A common approach is to apply displacement boundary conditions and evaluate the material's response.

Generating realistic three-dimensional fiber networks is a complex task due to the influence of topological entanglements, fiber geometry, and orientation distribution. Micheletti et al. [6], discussed the influence of spatial and topological constraints in determining the morphology and connectivity of filamentous systems, directly affecting their mechanical response. Picu [7] emphasizes that accurate modeling of random networks must capture not only the global orientation distribution but also local curvature, contact interactions, and network connectivity. Stochastic approaches based on random-walk algorithms, such as those presented by Altendorf and Jeulin [8],

provide a versatile computational framework to reproduce the statistical features of real fiber systems.

In this work, a persistent random walk with orientation sampling via the von Mises–Fisher distribution is employed, enabling controlled generation of fiber trajectories that respect curvature limits, avoid self-intersections, and match a prescribed volume fraction. The generated networks are embedded into a hyperelastic matrix and analyzed through finite element simulations to evaluate the influence of RVE size on the effective elastic response. The main objective is to establish a robust computational framework for generating physically consistent RFNs and to identify the minimum RVE size capable of accurately representing the macroscopic mechanical behavior of the studied composite.

2 Fiber Geometry Generation

2.1 Theoretical background

Realistic modeling of fiber geometry in three-dimensional networks requires representing stochastic and geometric aspects that reproduce both the variability of orientation and the curvature and connectivity of fibers in the matrix. This work adopts an approach based on persistent random walks with orientation control via the von Mises-Fisher (vMF) distribution.

The method follows the general guidelines for generating three-dimensional networks described by Micheletti et al. [3], in which the fiber trajectory is defined incrementally from an initial point and a unit direction vector, preserving correlation between consecutive steps. The implementation of self-avoidance and collision detection follows the geometric principles discussed by Picu [4], essential for avoiding fiber overlaps and ensuring microstructural representativeness.

2.2 Mathematical Formulation

The initial direction d_0 is sampled uniformly on the unit sphere $\mathbb{S}^2$. For each step k, the new direction d_k is obtained according to the vMF distribution:

$$f(x|\mu,\kappa) = C_p(\kappa)\, exp(\kappa\mu^T x), \tag{1}$$

where $\mu = d_{k-1}$ is the local mean direction, $\kappa \geq 0$ controls angular concentration, and $C_p(\kappa)$ is the normalization constant in $p = 3$ dimensions:

$$C_3(\kappa) = \frac{\kappa}{4\pi\, sin}. \tag{2}$$

When $\kappa \to 0$, the vMF converges to the uniform distribution on the sphere; high κ values restrict possible directions to a narrow cone around μ.

The next point p_k is computed as:

$$p_k = p_{k-1} + \Delta s d_k, \tag{3}$$

where Δs is the fixed step size.

To avoid intersection with existing fibers or with previous segments of the same fiber, the minimum distance between the new segment $\overline{p_{k-1}p_k}$ and each existing segment $\overline{AB}$ is computed:

$$d_{min} = \min_{s,t\in[0,1]} \|(p_{k-1} + su) - (A + tv)\|, \tag{4}$$

where $u = p_k - p_{k-1}$, and $v = B - A$. The segment is accepted only if:

$$d_{min} \geq 2r_f + \delta, \tag{5}$$

with r_f being the fiber radius and δ a safety margin.

If p_k exceeds the RVE limits, fiber growth is interrupted, allowing truncated fibers at the boundary, as discussed by Altendorf & Jeulin [5] to represent interactions with adjacent volumes.

After generating all fibers, the resulting volume fraction (VF) is:

$$\phi_{real} = \frac{\pi r_f^2 \sum_{i=1}^{N} L_i}{V_{box}}, \tag{6}$$

and the number of fibers is iteratively adjusted according to:

$$N_{new} = \frac{\phi_{target} V_{box}}{\pi r_f^2 \bar{L}}, \tag{7}$$

until $(\phi_{real} - \phi_{target})/\phi_{target}$ is below a predefined threshold.

2.3 Computational Procedure

The MATLAB implementation follows these steps:

- Parameter initialization – Define L_x, L_y, L_z, r_f, Δs, ϕ_{target} and κ.
- Initial estimate of N – Calculated using eq. (7) with $\bar{L} \approx L_f$.
- Fiber generation:
    - Choose a random initial point within the RVE.
    - The initial direction is uniform on $\mathbb{S}^2$.
    - At each step:
        - Generated a new direction via vMF centered on the previous one ($\mu = d_{k-1}$, parameter κ).
        - Apply the self-avoidance criterion (eq. (4) and eq. (5)).
        - If accepted, update the trajectory (eq. (3)).
        - If the point leaves the RVE, stop fiber growth.
- Iterative VF adjustment – After generating all fibers, recalculate N according to eq. (7) until convergence.
- Export and visualization – Fibers are saved in .csv files and visualized with distinct colors.

The export occurs for different lengths of RVE, according to need for the numerical analysis.

3 Theoretical RVE Formulation

In multiscale theory, it is considered that the microscopic displacement field $u(X,t)$ and the macroscopic deformation gradient $F(X,t)$ are related to the microscale through the volume average of their respective microscopic fields $u_\mu(Y,t)$ and $F_\mu(Y,t)$, according to:

$$u(X,t) = \frac{1}{V_\mu} \int_{\Omega_Y} u_\mu(Y,t) dV_\mu, \tag{8}$$

and

$$F(X,t) = \frac{1}{V_\mu} \int_{\Omega_Y} F_\mu(Y,t) dV_\mu, \tag{9}$$

where V_μ represents the reference volume of the RVE. The mappings presented in eq. (8) and eq. (9) are referred to as homogenization operations [6].

The deformation gradient F is a second-order tensor composed of partial derivatives relating changes in the deformed configuration to the undeformed configuration:

$$F_{ij} = \frac{\partial x_i}{\partial X_j}, \tag{10}$$

Other useful measures include the right and left Cauchy-Green tensors,

$$C = F^T F; \qquad b = F F^T. \tag{11}$$

Hyperelastic materials are commonly modeled through a strain energy density function Ψ, which is a scalar function of a deformation measure, such as F:

$$\Psi = \Psi(F), \tag{12}$$

The value of the strain energy function must remain invariant under the choice of deformation measure.

Moreover, the relation between stress and strain is given by:

$$P = \frac{\partial \Psi(F)}{\partial F}, \tag{13}$$

where P is the first Piola-Kirchhoff stress tensor.

Alternative stress measures include the second Piola-Kirchhoff stress tensor:

$$S = 2\frac{\partial \Psi(C)}{\partial C}, \tag{14}$$

and the Cauchy stress tensor:

$$\sigma = \frac{1}{J} FSF^T, \tag{15}$$

By Hill's theorem, equilibrium is satisfied in the absence of body forces. Thus, the stress tensor satisfies:

$$\sigma_{ik} = \left(\sigma_{ij} x_k\right)_{,j}, \tag{16}$$

and the average stress field in the material can be expressed as:

$$\langle \sigma_{ij} \rangle_\Omega = \frac{1}{|\Omega|} \int_\Omega \left(\sigma_{ik} x_j\right)_{,k} d\Omega, \tag{17}$$

Applying Green's Theorem and recognizing that Γ is the external boundary of the matrix, the average stress field can be written as:

$$\langle \sigma_{ij} \rangle_\Omega = \frac{1}{|\Omega|} \int_\Gamma \sigma_{ik} x_j n_k \, d\Gamma, \tag{18}$$

where n_k is the outward normal. This average stress is known as the Cauchy stress, from which the second Piola-Kirchhoff stress tensor can be obtained. This tensor is then used to determine the constitutive tensor $\mathbb{C}_{IJKL}$ which, in the case of a composite material, corresponds to the effective properties of the homogenized medium. The components of this tensor can be obtained using [7]:

$$\mathbb{C} = 2\frac{\partial S(C)}{\partial C} \qquad or \qquad \mathbb{C}_{IJKL} = 2\frac{\partial S_{IJ}}{\partial C_{KL}}. \tag{19}$$

4 Materials

The base material is room-temperature vulcanized (RTV) silicone rubber. A two-term Mooney-Rivlin model [7,8] was considered to characterize the matrix. The parameters considered were $C_{10} = 0.25MPa$, $C_{01} = 0.05MPa$, and $J = 1$, assuming incompressibility.

Polyester fiber was used as reinforcement. Their mechanical properties are listed in Table 1.

Table 1. Mechanical properties of polyester (PES).

	Unit	Value
Young's modulus E	GPa	3.0
Poisson's ratio ν	-	0.38
Density	kg/m³	1390

5 Finite Element Modeling

For this study, a fiber volume fraction of 20% was considered, with a fiber length of $l = 30mm$ and a diameter of $d = 50\mu m$. Additionally, 10 geometry sample were generated for finite element analysis. The RVE size was varied from 1mm to 4mm, with an increment of 0.5mm.

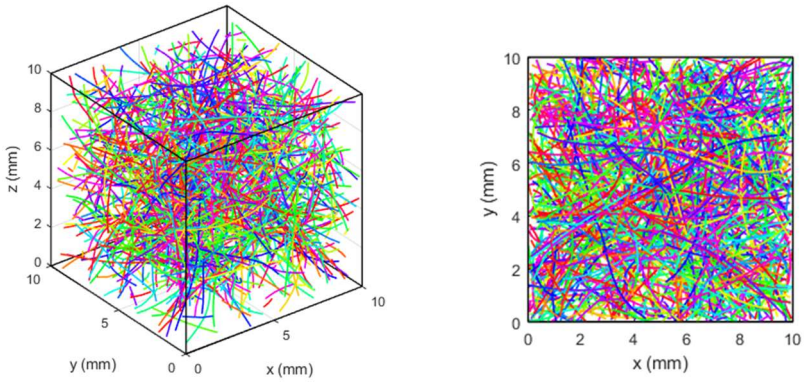
The geometries are imported into ANSYS [8] and incorporated into the matrix (SOLID185) using the REINF264 reinforcement element. A 0.1mm mesh (MESH200) was used. The boundary conditions defined for the analysis consist of three simply supported faces, one per axis, and a prescribed displacement $u_1 = L/10$

resulting in a uniaxial stretch of $\lambda_1 = 1.1$.

As outputs, normal and shear stresses and nodal coordinates on the surface were extracted. From the Cauchy stress, the second Piola-Kirchhoff stress tensor and $\mathbb{C}_{1111}$ were computed.

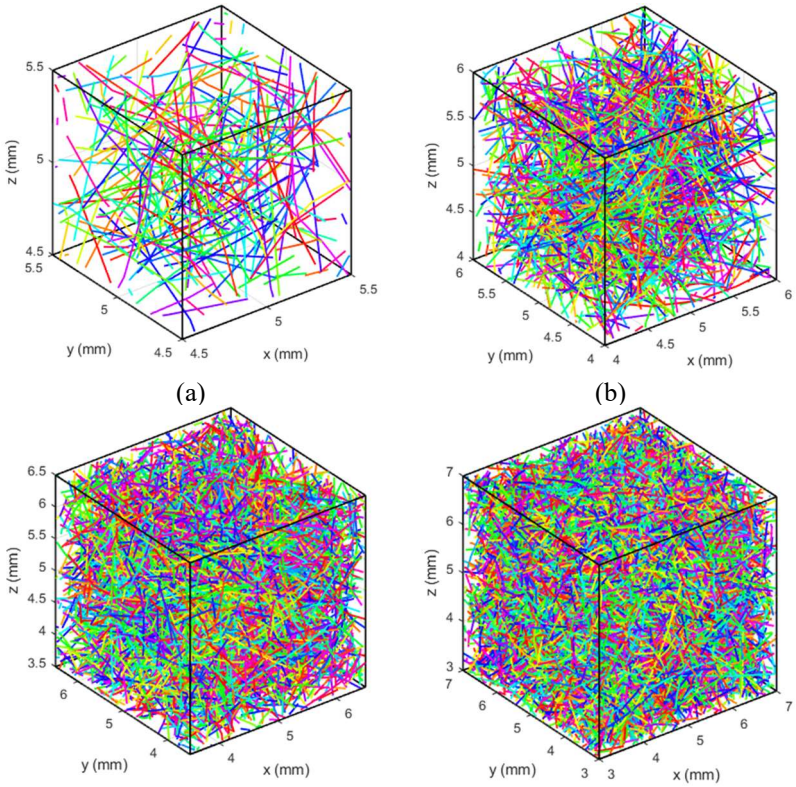
6 Results and Discussions

The Figure 2 shown an example of fiber geometry generated in MATLAB, for the case of $L_x = L_y = L_z = 10mm$ and $\phi_{target} = 3\%$, these values are defined as example due to visibility of random walk of fibers are major than $\phi_{target} = 20\%$ used in the numerical simulations, whose RVEs are shown in Figure 3.



(a) (b)

Figure 2. Example of fiber geometry generated with $L_x = L_y = L_z = 10mm$ and $\phi_{target} = 3\%$ (a) 3D, and (b) xy projection



(a) (b)

(d) (e)

Figure 3. Chosen RVE sizes (a) 1mm, (b) 2mm, (c) 3mm, and (d) 4mm.

After completing all analyses, obtaining the results, and calculating the material elasticity tensor following

the steps outlined in the methodology, the graphs presented in this section were plotted. Figure 4 shows the results obtained for the RVE with L = 3,5mm, illustrating the 10 values of $\mathbb{C}_{1111}$ obtained. Figure 5 presents the results for all simulations carried out, varying the RVE size length and the fiber numbers, as show here.

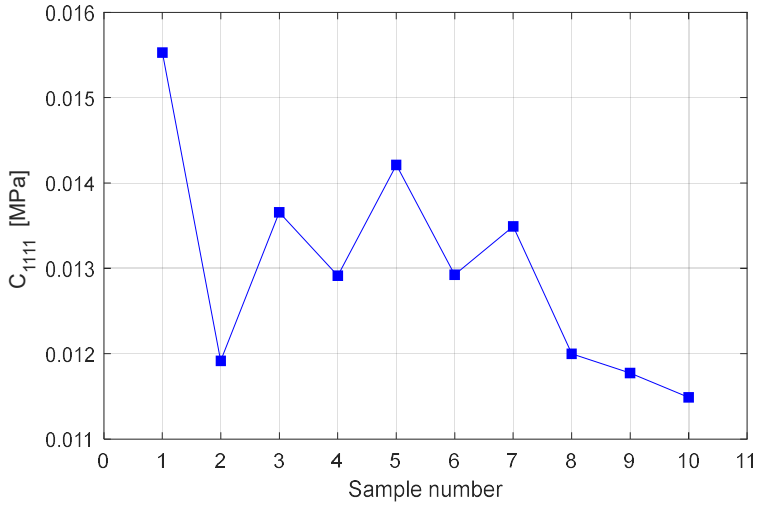


Figure 4. Material elastic property for case of $L = 3.5mm$.

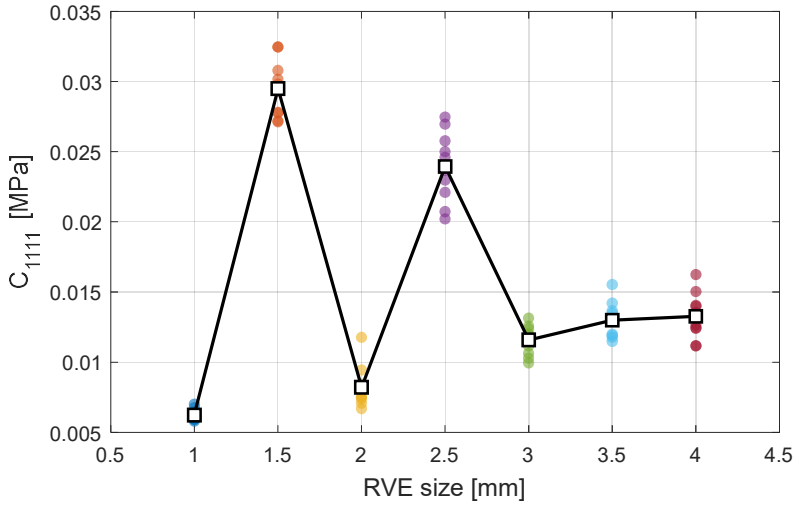


Figure 5. Fiber number vs. material elastic property homogenized.

From the curve in Figure 5, and considering the proximity of the values obtained for the various samples analyzed, it is possible to observe a convergence trend starting at $L = 3.5mm$, indicating that this is the minimum RVE size suitable for representing the effective properties of the material.

7 Conclusions

This work presented a computational formulation for generating three-dimensional random fiber networks based on persistent random walks with orientation via the von Mises-Fisher distribution. The algorithm incorporates curvature control, self-avoidance, and collision detection, ensuring realistic fiber arrangements within a cubic Representative Volume Element (RVE). The method allows precise control of geometric parameters such as fiber length, radius, target volume fraction, and orientation correlation, while maintaining geometric continuity and avoiding overlaps.

The proposed approach offers significant advantages for micromechanical modeling, including direct generation of closed and consistent geometries ready for import into a software of finite elements without need for post-processing or geometry repair.

Application to RVEs of varying sizes demonstrated the method's ability to support convergence studies of effective elastic properties. Convergence of the homogenized modulus $\mathbb{C}_{1111}$ was observed for RVE sized above 3.5mm, indicating a suitable minimum domain size for capturing the macroscopic mechanical response.

These results will serve as the foundation for future work aimed at deriving the constitutive equation of the anisotropic hyperelastic material, taking into account fibers generated through a random walk. For this purpose, the method will be applied to multiple loading conditions, anisotropic matrix-fiber interactions, and alternative fiber volume fractions.

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