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Research Article

Parametric Framework for the Modeling and Generation of Nanofibrous Structures

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ABSTRACT

Nanofibrous structures are widely used in filtration, membrane separation, protective materials, biomedical systems, and other transport-related applications. Numerical simulation of flow and transport phenomena in such media requires a reliable geometrical representation of the fibrous domain. However, generating controlled fibrous geometries, particularly random and disordered structures with prescribed fiber diameter, orientation, and density, remains a challenging and time-consuming step in computational modeling. In this study, a MATLAB-based computational code coupled with COMSOL Multiphysics through Live-Link is developed to generate micro/nanofibrous structures inside a cylindrical computational domain. The proposed framework enables the construction of a single fiber with arbitrary dimensions, arrays of parallel fibers, fibers with prescribed orientations, and fully random fibrous networks. The code allows independent control over key structural parameters, including fiber diameter, fiber number, fiber density, orientation, spatial distribution, and computational domain size. Moreover, fibrous structures can be generated using uniform or non-uniform fiber diameters, making the method suitable for representing both idealized and more realistic fibrous media. The generated geometries can be directly used in COMSOL Multiphysics as initial computational domains for the simulation of fluid flow, pressure drop, permeability, particle transport, and other coupled physical phenomena. The developed MATLAB–COMSOL Live-Link framework provides a flexible and efficient tool for rapidly constructing parametric fibrous geometries and systematically studying the effect of microstructural parameters on transport behavior in fibrous media. This approach can facilitate the design, optimization, and numerical analysis of micro/nanofibrous materials in filtration and related applications.

1. Introduction

Nanofibrous structures have attracted considerable attention in various scientific and engineering fields in recent years due to their high specific surface area, high porosity, tunable architecture, and the ability to achieve multifunctionality [1-4]. These unique characteristics make them exceptionally promising for a wide range of applications, including tissue engineering [5-8], drug delivery [9-12], filtration [13-18], energy storage [19-22], and sensors [23-25]. The high specific surface area of these fibrous materials significantly enhances their interaction with surrounding environments, which is crucial for applications such as catalysis and adsorption [26]. Moreover, their high porosity facilitates efficient mass transport and cell infiltration, making them ideal scaffolds for regenerative medicine [27]. The tunable architecture of nanofibers allows researchers to precisely control their mechanical

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properties, degradation rates, and biological responses, enabling the design of customized materials for specific biomedical applications [28-30]. Furthermore, the ability to achieve multifunctionality by incorporating various functional components, such as drugs, growth factors, and conductive polymers, into the fibrous structures opens up new possibilities for advanced therapeutic strategies and smart materials [31, 32]. As a result, these fibrous materials have become a focal point of interdisciplinary research, bridging the gap between materials science, biology, and engineering [33]. The ongoing development of novel fabrication techniques, such as electrospinning and self-assembly, has further expanded the potential of these structures, allowing for the creation of complex and hierarchical architectures that mimic natural extracellular matrices [27, 34, 35].

Nanofibrous structures are poised to play a pivotal role in addressing critical challenges in healthcare, environmental sustainability, and energy technologies [36]. Therefore, investigating various transport and mechanical phenomena within fibrous structures has emerged as a cornerstone of contemporary materials science and engineering [37, 38]. Understanding the intricate interplay between fluid dynamics, heat transfer, and particle deposition within these media is essential for optimizing their performance and longevity [39-41]. As industries shift towards nanotechnology and precision manufacturing, the ability to accurately predict how nanofibrous networks behave under multi-physical conditions becomes indispensable. Consequently, researchers are increasingly focused on deciphering the relationship between the stochastic nature of fiber arrangements and their macroscopic functional properties. This pursuit not only drives the development of more resilient and efficient materials but also necessitates the creation of sophisticated computational tools capable of bridging the gap between theoretical modeling and real-world experimental observations.

Researchers have conducted different approaches, including analytical methods, experimental techniques, and computer simulations for that [42]. Traditional analytical models, owing to simplifying assumptions such as ordered and two-dimensional fiber arrangements, are unable to predict the behavior of realistic random and three-dimensional structures [43, 44]. On the other hand, conducting experimental tests for all possible combinations of structural parameters such as fiber diameter, density, and orientation is extremely costly and time-consuming, and in many cases impractical [45, 46]. In contrast, numerical simulation enables systematic and controlled investigation of the effect of each parameter independently on transport phenomena such as pressure drop and collection efficiency [47-49]. Particularly at the nanoscale, phenomena such as the slip effect, which occurs due to the proximity of fiber diameter to the molecular mean free path, cannot be directly measured and can only be analyzed through numerical modeling with appropriate boundary conditions [50]. Ultimately, numerical modeling significantly reduces the need for costly experimental tests, accelerates the optimization and design process of new structures, and enables performance prediction prior to prototype fabrication [51]. Two-dimensional models had limitations and were unable to fully address three-dimensional phenomena [52]. Over time, researchers gradually moved toward three-dimensional and random modeling. A dedicated C++ code, were the first to model three-dimensional spun-bonded structures using the μ-randomness algorithm without fiber interpenetration [47]. That research subsequently extended to the short fibers using the I-randomness algorithm [48]. Another approach involved modeling structures with controlled fiber orientation that generated three-dimensional structures with normal distributions for in-plane and through-plane angles [53]. In recent years, new methods have been introduced, including the use of commercial software such as COMSOL Multiphysics, for directly designed three-dimensional structures with varying fiber diameters within the software environment [54]. Additionally, image-based approaches utilizing three-dimensional reconstruction from SEM or XMT images in software such as Avizo and GeoDict [51, 55]. Alongside these methods, modeling using dynamic contact simulation in Abaqus has also been proposed for generating more realistic structures [56]. Despite the diversity of these approaches, many suffer from limitations such as high computational cost, dependence on high-quality images, lack of complete control over structural parameters, or inability to directly integrate with flow simulation software [57].

In this study, by developing a code in MATLAB (2023b) and utilizing the Live-Link capability to COMSOL Multiphysics (6.2.2) we have attempted to provide a platform that, while benefiting from MATLAB's flexibility in generating random and controlled geometries, enables direct and real-time transfer of the generated structure to COMSOL for simulation of various physical phenomena. This code is capable of generating a wide range of structures—from a single fiber in a cylindrical domain to fully random networks with control over the number, density, and diameter distribution of fibers—and significantly overcomes the limitations of previous methods.

2. Method

In this study, a custom MATLAB code has been developed and integrated with COMSOL Multiphysics through the Live-Link interface, enabling seamless and real-time transfer of the generated geometries to the simulation environment. The program requires the user to define key input parameters, including the overall dimensions of the computational domain, fiber diameter, the number of fibers, and their statistical distribution. Based on the user's selection, the algorithm subsequently generates either ordered (e.g., parallel or layered arrays) or random (e.g., disordered networks) fibrous structures within the specified domain. The final constructed geometry is automatically exported to COMSOL, where it is visualized and can be directly utilized for subsequent physical simulations, such as fluid flow, particle transport, or heat transfer analysis. The complete set of controllable parameters incorporated in the present algorithm is summarized in Table 1.

Table 1. Adjustable Parameters of the Algorithm of the Fibrous Generation.

Category	Description
Domain	Domain dimenssions
	Number of fiber layers
Fiber	Fiber diameter
	Probability distribution of Fiber diameter
	Minimum and Maximum fiber length
	Inter-fiber distance
	Fiber's distance from boundaries
	Maximum placement attempts
	Number of fiber placement

In this code, the geometric constraints of the domain, including the radius, height, and specified margins around the lateral walls as well as the top and bottom surfaces, are strictly enforced. This ensures that no fiber exits the domain boundaries, and the inter-fiber distances are maintained within the prescribed minimum and maximum limits, thereby preventing any unwanted overlap between fibers. The probabilistic distribution implemented in the code allows for the presence of both large and small fibers with a specified density within the final structure. The algorithm proceeds in a layer-by-layer manner, such that each layer has a designated central height within the domain, and the fibers are generated around this height. This approach ensures that the fibers are stacked on top of each other in a layered arrangement without crossing the top or bottom boundaries.

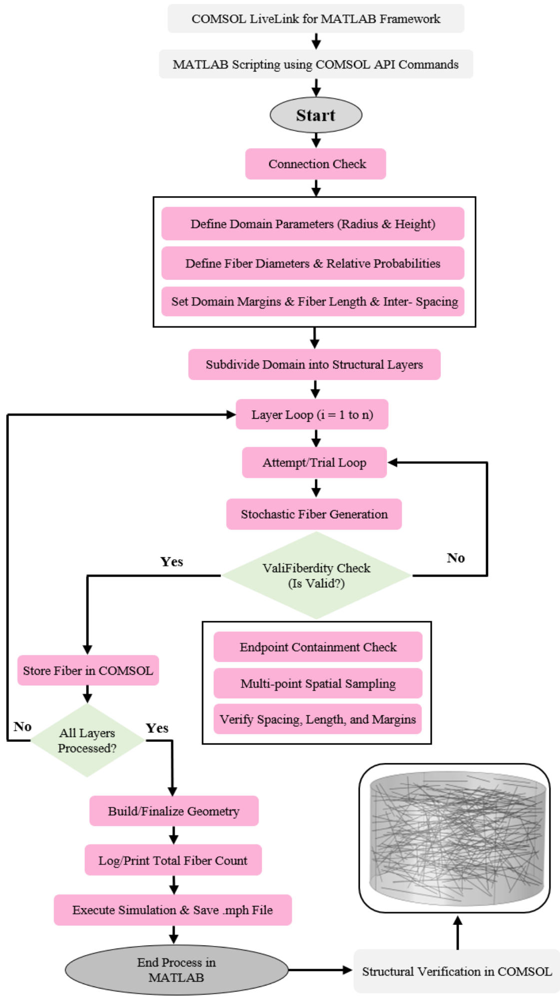

Fig. 1. Flowchart of three-dimensional fibrous structure generation within a cylindrical domain, organized in a layered manner in MATLAB while its output automatically transferred to COMSOL.

For each fiber, the algorithm first randomly selects its three-dimensional center, orientation, and length. Following the initial selection, auxiliary functions are employed to verify that the entire fiber length lies within the domain and that no point of the fiber violates the walls or the top/bottom surfaces. Additionally, the new fiber is checked for overlap with other fibers already existing in the same layer and, if necessary, with those in adjacent layers, ensuring that the inter-fiber distances conform to the specified minimum and maximum thresholds. Only those fibers that satisfy all geometric and spatial constraints are added to the domain. The flowchart in Figure 1 illustrating the graphical representation of the algorithm's workflow demonstrates the decision-making steps, random sampling, geometric and spatial constraint verification, and the collision control process in a simplified manner.

All steps of the geometry generation processes were carried out on a standard desktop computer featuring a 12th generation Intel Core i7-12700H processor (14 physical cores, 20 threads, base clock speed of 2.30 GHz) and 16 GB of RAM. The program's runtime for generating simple geometries was consistently under one minute, whereas more complex fibrous structures required less than three minutes to complete the generation and export procedures.

3. Results

In this study, a MATLAB code was developed and linked to COMSOL Multiphysics through the LiveLink interface to enable the generation of a wide variety of fibrous structures within a cylindrical computational domain.

3.1. Simple Fibrous Structures

This code is capable of generating various configurations of fibrous networks. The figure shows the COMSOL outputs corresponding to (a) single fibers, (b) planar arrangement, (c) angular arrangement, (d) aligned planar fiber arrangement with fibers tangent to each other, (e) orthogonal planar fiber arrangement with fibers tangent to each other, and (f) 45° angular planar fiber arrangement with fibers tangent to each other, all within the same computational domain. The computational domain is a cylinder with a diameter and height of 5 µm, and the fiber diameter is set to 100 nm. As can be observed, none of the fibers protrude outside the domain.

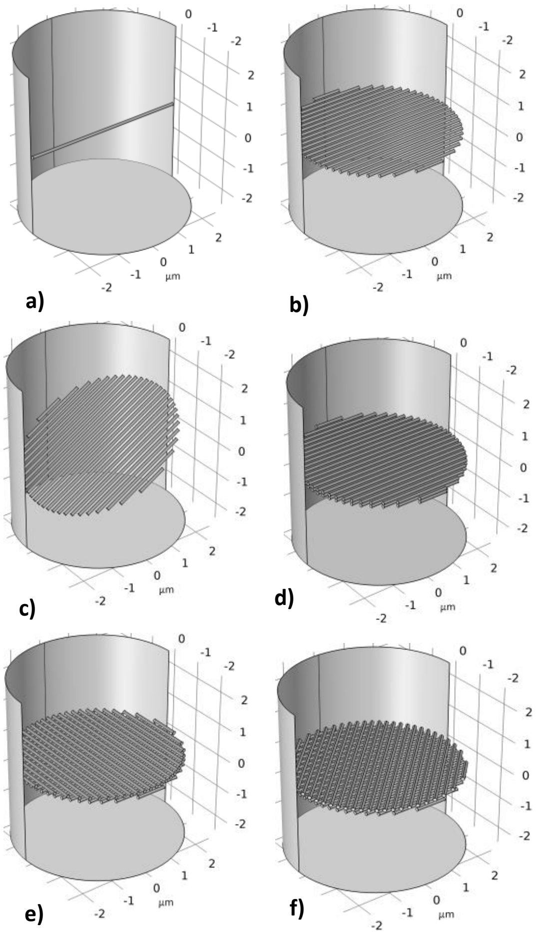

Fig. 2. Simple fibrous structures: (a) single fiber, (b) planar arrangement, (c) angular arrangement, (d) aligned planar fiber arrangement with fibers tangent to each other, (e) orthogonal planar fiber arrangement with fibers tangent to each other, and (f) 45° angled planar fiber arrangement with fibers tangent to each other. The computational domain is a cylinder with a diameter and height of 5 µm. The fiber diameter is set to 100 nm.

3.2. Random Fibrous Structures

The developed code enables the generation of highly disordered fibrous structures with controllable packing densities. Figure X presents examples of fibrous structures produced with low, medium, and high packing densities. It should be noted that the packing density can be defined even more densely depending on the specific application requirements. As clearly illustrated in the figure, increasing the packing density results in a greater number of fibers per unit volume, which in turn enhances the degree of fiber entanglement and interpenetration within the network.

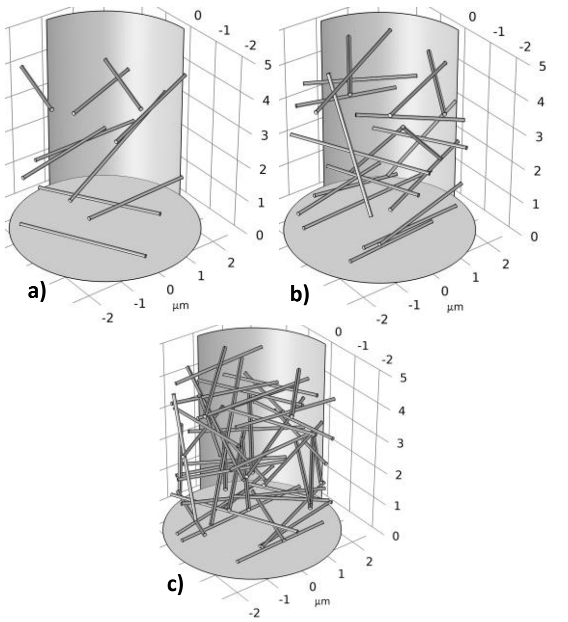

Fig. 3. Fibrous networks generated at different packing densities: (a) low, (b) medium, and (c) high. All dimensions are in micrometers. The fiber diameter is 100 nm

3.3. Controlled Random Structures

The geometry generation procedure is formulated such that the spatial positioning and orientation of the fibers are governed by controlled stochastic functions. As a result, each run of the code generates a distinct and unique fibrous microstructure, while the remaining geometric parameters—including the domain size, number of layers, and fiber diameter—are kept constant. The figure presents the random fibrous structures obtained from three independent executions of the code for a fiber diameter of 100 nm. In these structures, random configurations have been generated for a constant fiber density per unit volume. The results reperesent significant variations in the spatial arrangement, inter-fiber distances, and void regions across the independent runs. From a physical perspective, this behavior is in excellent agreement with real nanofiber media, particularly for electrospinning approches. Thus, the model is capable of reproducing this natural stochasticity while keeping constant porosity.

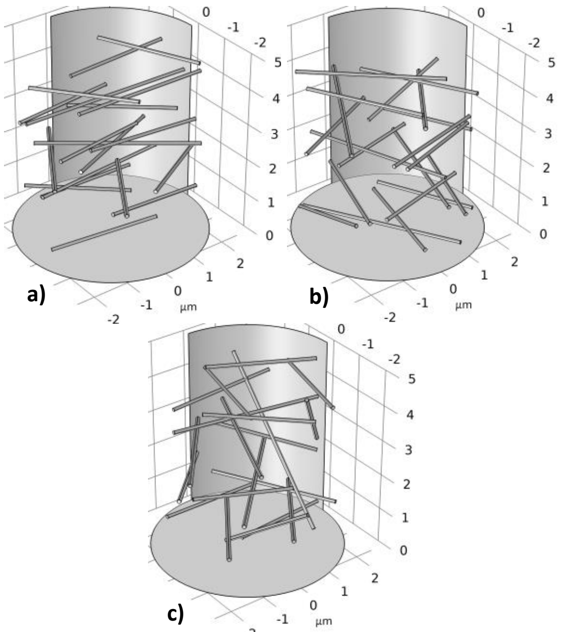

Fig. 4. Representative random nanofibrous structures generated under identical conditions, including the same computational domain dimensions, fiber diameter, and number of layers: (a) Run 1, (b) Run 2, and (c) Run 3.

3.4. Reproducibility and Parametric Control

A significant challenge in the fibrous networks modeling lies in the inability to reproduce a specific configuration consistently across multiple run of the algorithm. To address this, the present work incorporates a "Fixed Random Seed" mechanism, which enables the spatial distribution and orientation of fibers to be stored and retrieved independently of other parameters. Consequently, each stochastic parameter can be maintained constant across different runs while systematically varying a given parameter. As an example, the figure presents the results of two independent runs of the same random structure, where only the fiber diameter has been modified. It is evident that all random parameters are preserved between the two generated samples, with the sole variation being the fiber diameter. This capability facilitates the isolated investigation of the influence of fiber diameter on the physical phenomena of interest within an inherently random network.

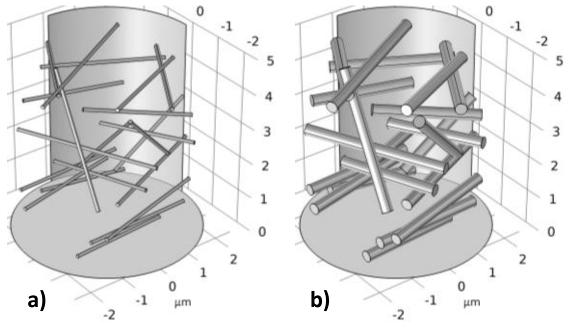

Fig. 5. Demonstration of reproducibility and independent parametric control. (a) Random fibrous structure generated with a fiber diameter of 100 nm, (b) generation of the identical random structure with a fiber diameter of 300 nm, while the spatial positions of the fibers are preserved from the previous case.

3.5. Heterogeneous Fiber Diameter

In this algorithm, the capability to define a heterogeneous distribution for fiber diameters has been incorporated to generate fibrous structures. This feature allows the creation of a network consisting of fibers with varying sizes, thereby resulting in a structure with greater geometric diversity. The figure presents the structures corresponding to three different fiber diameters, each assigned with a distinct probability of occurrence for its respective diameter range. Accordingly, during fiber generation, the fiber diameters is selected based on its assigned probability. Details of diameters and probabilities are listed in tables 2 and 3.

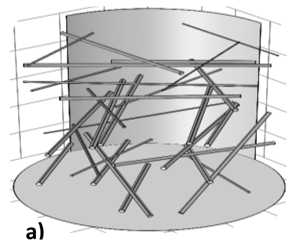

Table 2. Parameters

Fiber diameter (nm)	Probability (%)
25	20
50	30
100	50

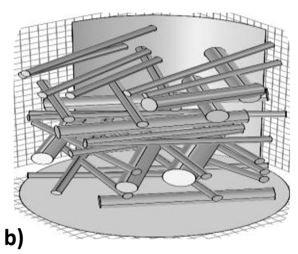

Table 3. Parameters

Fiber diameter (nm)	Probability (%)
1000	20
2000	30
3000	50

Fig. 6. Fibrous structure with heterogeneous fiber diameter distribution. The fiber diameter distribution and corresponding probability of occurrence within the fibrous structure are shown in the table alongside each case.

3.6. Geometric Scalability

One of the key features of the algorithm presented in this study is the flexibility in defining the dimensions of the computational domain without any limitation on the number of fibers or geometric complexity. As illustrated in Figure 1, the algorithm is capable of generating fibrous structures within cylindrical domains of varying heights and diameters while maintaining the physical parameters, such as the fiber diameter (100 nm).

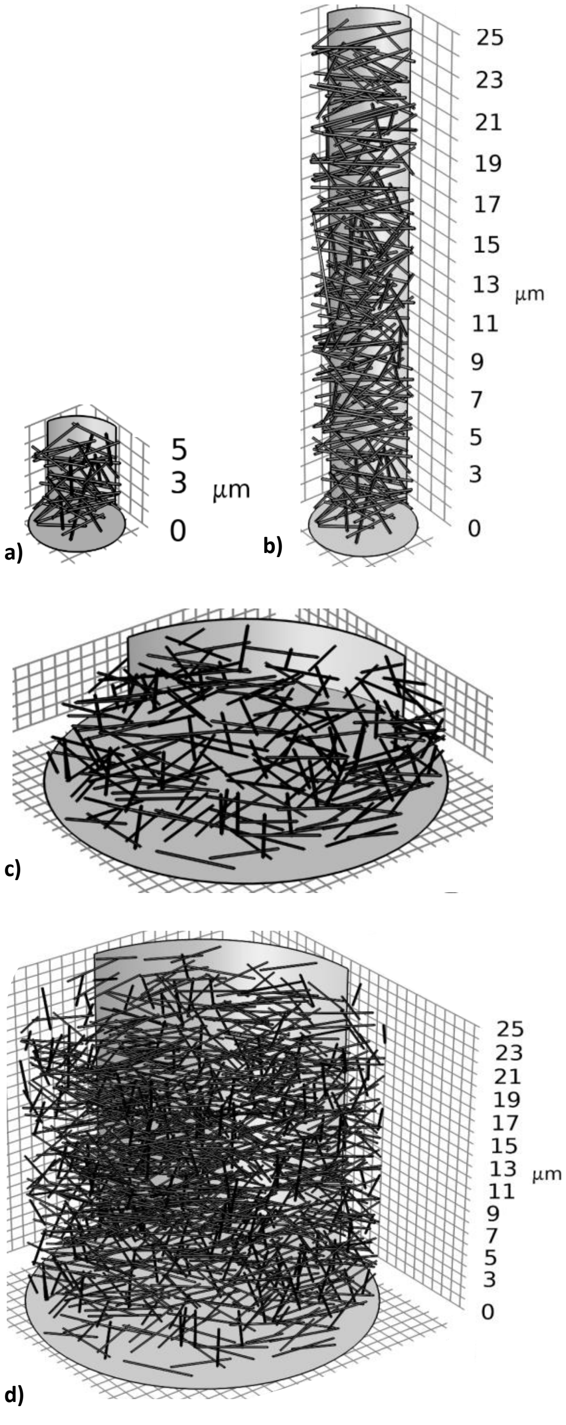

Fig. 7. Generation of cylindrical computational domains with variable dimensions with the same fiber density. a) diameter 5 µm, height 5 µm, b) diameter 5 µm, height 25 µm, c) diameter 25 µm, height 5 µm and d) diameter 25 µm, height 25 µm. The fiber diameter is set to 100 nm for all generated fibers.

In this work, a MATLAB-based parametric code was developed and interfaced with COMSOL Multiphysics through the Live-Link connection, enabling the automated and rapid generation of three-dimensional fibrous structures within a cylindrical computational domain. The core novelty of the presented algorithm lies in its ability to produce a broad spectrum of fiber configurations—from isolated single fibers and ordered planar arrays to fully stochastic three-dimensional networks—while offering the user independent control over key geometric parameters including fiber diameter, packing density, layer count, and spatial orientation. A distinctive feature of the code is its capacity to maintain exact reproducibility across different simulation runs through the implementation of a fixed random seed, which preserves the spatial coordinates and orientation of fibers even when other geometric attributes are modified. This functionality enables systematic and isolated parametric studies, where the influence of a specific structural variable—such as fiber diameter or domain size—can be investigated without the confounding effect of randomness. Additionally, the algorithm supports heterogeneous fiber diameter distributions, allowing for the generation of multi-scale networks with controlled statistical properties, which are essential for mimicking realistic electrospun nonwoven materials. The geometry generation process is organized in a layer-by-layer fashion, ensuring that fibers are placed within the domain boundaries while respecting prescribed minimum and maximum inter-fiber distances, thereby preventing unwanted overlaps. The computational efficiency of the code was demonstrated on a standard desktop system, with generation times of less than one minute for simple configurations and under three minutes for complex, highly dense networks. The seamless integration with COMSOL via Live-Link eliminates the need for intermediate file conversions, significantly streamlining the workflow from geometry generation to physical simulation. This direct coupling allows for immediate investigation of transport phenomena such as fluid flow, particle deposition, and heat transfer within the generated fibrous structures, making the tool particularly valuable for optimizing filter media design and other applications requiring precise microstructural control. Future developments will focus on extending the algorithm to incorporate curved and helical fiber morphologies, as well as enabling the generation of graded and functionally graded structures. The framework presented here provides a robust and versatile platform for bridging the gap between microstructural design and macroscopic performance prediction in fibrous materials.

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