Development and validation of optimized multiscale structures in 3d-printed polymers: an integrated simulation and experimental approach

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Abstract. This study proposes an integrated workflow that combines topology optimization, numerical simulation, and additive manufacturing for the development and validation of polymer structures subjected to bending. The methodology employs the SIMP method to redistribute material within structural models, with the results converted into lattice geometries using a Diamond-type unit cell. Finite Element Analysis is used to simulate the mechanical behavior of the optimized geometries, while fabrication is carried out through Fused Deposition Modeling using PLA filament. The specimens are then experimentally evaluated through three-point bending tests, allowing for validation of the computational model. The results show that the optimized structure exhibits higher specific stiffness and mechanical behavior influenced by the geometric characteristics of the lattice. The good correlation between simulated and experimental data in the elastic region validates the adopted approach, while the discrepancies observed in the post-yield phase reflect the effects of printing-induced anisotropy, geometric imperfections, and simplified constitutive modeling. This work highlights the potential of topology optimization combined with additive manufacturing as an effective strategy for designing lightweight components, while also emphasizing the challenges related to accurately predicting the mechanical behavior of complex structures.

Keywords: Topology Optimization, Additive Manufacturing, Lattice Structures, Fused Deposition Modeling, Polylactic Acid, Finite Element Analysis.

1 Introduction

The search for lightweight and high-performance structural components drives advances in fields such as aerospace, automotive, and biomedical engineering [1]. Mass reduction is directly related to lower operational costs, increased energy efficiency, and improved dynamic behavior of systems [2]. In this context, Topology Optimization (TO) has emerged as a powerful computational engineering tool, enabling efficient material distributions that maximize structural stiffness or other performance criteria for a given available volume [3,4].

The application of TO is carried out using the Finite Element Method (FEM), which provides the foundation for numerically assessing the structural response of optimized geometries [1]. Through FEM, it is possible to simulate stress, displacement, and strain energy fields, allowing optimization algorithms to iterate over different material distributions until an ideal configuration is achieved [5]. This integration between FEM and TO enables the development of highly efficient components, with mass reductions that can enhance structural performance when compared to conventionally designed geometries [6].

With the advancement of Additive Manufacturing (AM), particularly Fused Deposition Modeling (FDM), it has become possible to fabricate complex geometries derived from TO, overcoming the limitations of traditional methods such as machining and casting [7]. Layer-by-layer 3D printing allows for the realization of organic and highly optimized topologies, bridging the gap between computational design and practical application.

In this study, FDM technology is employed using Polylactic Acid (PLA) filament, selected for its wide availability, low cost, and biodegradable nature. Despite these advantages, FDM introduces significant mechanical anisotropy due to layer orientation, with property variations that can exceed 50% depending on the printing direction [8]. This anisotropy imposes relevant limitations on the accuracy of FEM-based simulation models, which commonly assume isotropic material behavior [9].

Therefore, the objective of this study is to design and simulate PLA beams via FEM, fabricate them using FDM, and experimentally validate their flexural behavior, considering both non-optimized and topology-optimized models. The comparative analysis aims to evaluate the structural benefits of TO and the fidelity of numerical modeling considering the challenges posed by the anisotropy introduced by the manufacturing process.

2 Materials and methods

This section details each stage of the design, manufacturing, simulation, and testing process to ensure full reproducibility of the study. The choice of parameters is justified based on technical standards, literature, and project-specific data.

2.1 Finite Element Modeling

Numerical analyses were performed in the Static Structural module of Ansys 2025 R1 [10]. A nonlinear static analysis was carried out, with the "Large Deflection" option enabled. This choice is crucial to accurately capturing the geometric nonlinear effects that arise from the large displacements observed in flexural tests of ductile polymers [9].

The solid specimen was discretized using hexahedral elements, while the complex geometry of the optimized beam required a finer and adaptive mesh composed of second-order tetrahedral elements (TET10). This higher-order mesh is essential to accurately capture stress gradients and curvatures at the lattice strut junctions, which are critical locations for the initiation of failures [9].

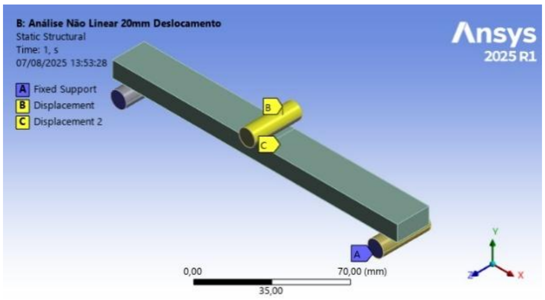

Figure 1 – Boundary conditions applied to the geometry.

As shown in Fig. 1, the boundary conditions were defined to accurately replicate the three-point bending test setup: two cylindrical supports at the base were modeled with displacement constraints (fixed supports), and a prescribed displacement was applied to a central line on the upper surface of the beam.

A fundamental aspect of the simulation was the material model. Based on experimental data, a custom material named "PLA BRANCO IFES" was created in Ansys using a multilinear isotropic plasticity model. This model allows the representation of plastic yielding and strain hardening of the material beyond the elastic limit.

2.2 Topology Optimization

The optimization was carried out in the Topology Optimization module of Ansys 2025 R1, which employs the SIMP (Solid Isotropic Material with Penalization) algorithm [1]. The optimization objective was formulated to minimize compliance (i.e., maximize overall stiffness) under a three-point bending load case, replicating the conditions of the experimental test. The main constraint was a target mass reduction, aiming to arbitrarily remove 30% of the material, as shown in Fig. 2.

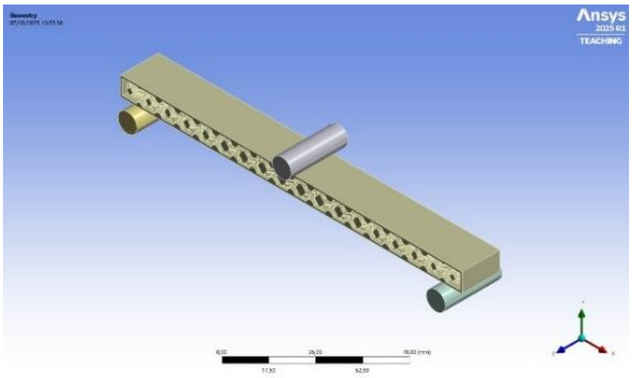

Figure 2 – Optimized beam with Diamond-type lattice structure.

A Diamond-type unit cell (Octet 1) with a size of 10 mm was selected. The local density of the lattice, controlled by the strut thickness—which corresponds to the cell edges—was adjusted to range between 30% and 90%, reflecting the optimized density contour: regions of higher density result in thicker struts, and vice versa [11]. This process, performed entirely within the Ansys environment, represents a multiscale approach in which macroscale optimization dictates the local microstructure [12]. The final lattice geometry was then exported for reanalysis and subsequent manufacturing.

2.3 Specimen Design

The base geometry of the specimen is a rectangular beam with dimensions of 180 mm in length, 20 mm in width, and 10 mm in height, modeled in Autodesk Inventor Professional 2025 [13]. These dimensions were selected to comply with ASTM D790 [14] for three-point bending tests, specifically targeting a span-to-thickness ratio of 16:1. This proportion is essential to ensure that failure occurs predominantly by bending, minimizing shear effects.

The material used was a commercial PLA filament with a diameter of 1.75 mm. PLA was chosen due to its popularity in FDM printing, low melting point—which reduces warping and residual stress and its biodegradable nature. As shown in Fig. 3, the specimens were fabricated on a Creality CR-10 V3 3D printer, manufactured by Shenzhen Creality 3D Technology Co., Ltd., with the G-code generated using PrusaSlicer 2.9.2 [15].

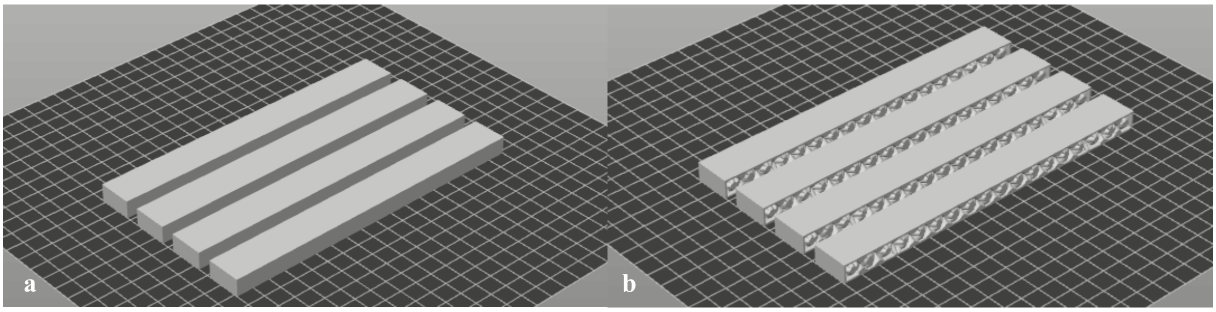

Figure 3 – Visualization of the specimens in PrusaSlicer. (a) Non-optimized beams; (b) Optimized beams.

The build orientation is a critical parameter that strongly affects the mechanical properties of printed parts. The specimens were printed in the flat orientation (XY-at), with the largest face parallel to the print bed. This choice was made to maximize flexural strength, as it aligns the long continuous filaments with the direction of tensile and compressive stresses, resulting in better mechanical performance compared to on-edge or upright orientations. The detailed printing parameters, essential for reproducibility, are summarized in Table 1.

Table 1. FDM Printing Parameters Used in the Fabrication of the Specimens

Parameter	Value	Justification
Material	PLA	Low cost, biodegradable, easy to print
Filament Diameter	1,75 mm	Commercial standard
Nozzle Diameter	0,4 mm	Standard for general-purpose printing
Layer Height	0,15 mm	Balance between resolution and printing time
Extrusion Temperature	190 °C	Within the recommended range for PLA
Bed Temperature	60 °C	Improves first-layer adhesion and reduces warping
Printing Speed	70 mm/s	Average speed to ensure quality and efficiency
Infill (Solid Specimen)	100% (Rectilinear)	To create a solid and fully dense baseline specimen
Build Orientation	Flat (XY-at)	Maximizes flexural strength by aligning filaments with the applied load

2.4 Flexural Test

Flexural tests were carried out on an EMIC JM universal testing machine, manufactured by Instron Brasil Equipment's Ltda., equipped with a 10 kN load cell, in strict accordance with ASTM D790. A custom testing fixture was used to ensure a free span of 162.5 mm between the lower supports, as specified by the standard for specimen geometry.

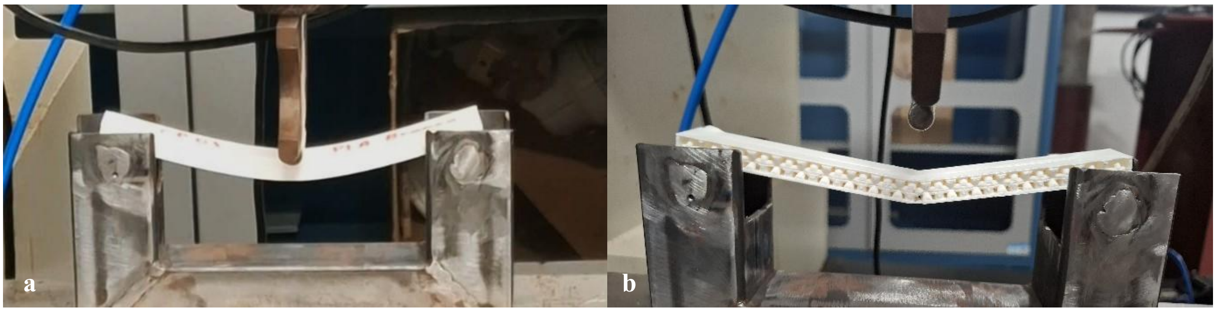

Figure 4 - Flexural test. (a) Non-optimized PLA beam under loading; (b) Optimized PLA beam under loading.

The test was conducted in a three-point bending configuration at a constant crosshead displacement rate of 5 mm/min, as shown in Fig. 4. During each test, applied force and mid-span displacement data were continuously recorded until complete fracture of the specimen. To ensure statistical reliability and assess the repeatability of the manufacturing process, four specimens were tested for each case, with and without optimization. The resulting data were subsequently organized and processed in spreadsheets [16].

3 Results and Discussion

This section compares structural performance, evaluates the correlation between simulation and experimental results, and discusses discrepancies considering the printing process and its implications for structural design.

3.1 Structural Performance Analysis: Force vs. Displacement

Measurements of the fabricated specimens revealed a 30% mass reduction for the optimized beam compared to the solid beam. Fig. 5 presents the simulated total displacement for both structural configurations, highlighting the stress redistribution caused by topology optimization.

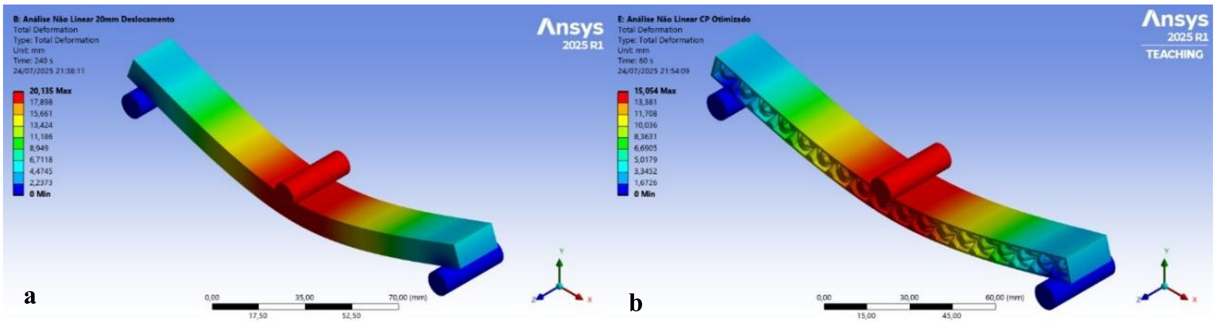

Figure 5 – Total displacement. (a) Non-optimized beam; (b) Optimized beam.

Fig. 6 shows the experimental and numerical force–displacement curves. For the non-optimized beam, the maximum measured load was 707.9 N at 20.1 mm displacement, while the simulation estimated 983.7 N. For the optimized beam, the experimental test recorded 317.9 N at 10.5 mm, compared to 408.2 N in the simulation. Good agreement is observed in the elastic region, with a relative error below 10% up to 8 mm for the solid beam and 11 mm for the optimized beam. After yielding, the model tends to overestimate the structural response due to material idealization and the absence of manufacturing imperfections.

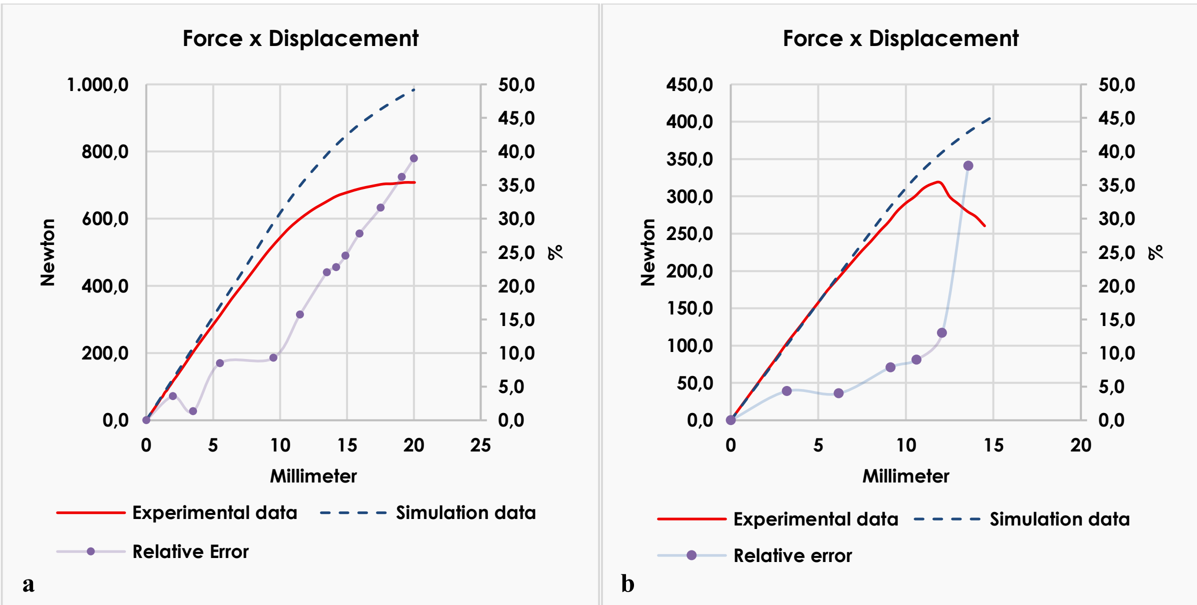

Figure 6 – Force vs Displacement curve. (a) Non-optimized beam; (b) Optimized beam.

The solid beam exhibited pronounced plastic yielding, with deformation distributed along its length prior to final fracture. In contrast, the optimized beam showed abrupt and localized failure, with fracture concentrated in the lower struts of the lattice structure—critical regions of maximum tensile stress. This behavior is characteristic of lattice-type structures, in which failure often initiates at nodes or thinner struts that act as stress concentrators [17]. These results indicate that topology optimization not only altered the material distribution but also changed the failure mode of the part, leading to a less ductile performance [19]. This observation is crucial for structural applications requiring energy absorption or deformation tolerance.

3.2 Structural Performance Analysis: Stress vs. Strain

Fig. 7 presents the stress analysis obtained from simulations for the solid and optimized beams. For both beams, the error between numerical and experimental results remained below 10% in flexural stiffness. In the case of the solid beam, this agreement is observed up to a displacement of 8 mm, while for the optimized beam it extends up to 11 mm. This discrepancy highlights the influence of the complex geometry and the anisotropic behavior of the lattice structure on the mechanical response.

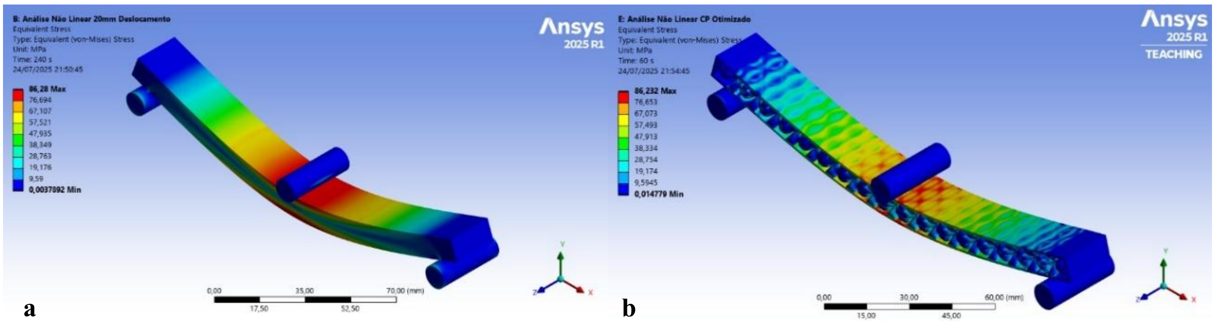

Figure 7 - Distribution of equivalent von Mises stresses (MPa) obtained from nonlinear simulation. (a) Non-optimized beam; (b) Optimized beam.

After yielding, the discrepancies between simulation and experiment become more pronounced. As shown in Fig. 6, the non-optimized beam exhibits an overestimation of load at higher displacements, while the optimized beam displays simulated stiffness and strength values higher than those observed experimentally, with delayed fractures. In Fig. 8, it is noted that the optimized beam reaches higher stress levels despite failing at a lower actual strain. These discrepancies stem from the idealization of the material as isotropic and the absence of geometric imperfections, indicating the need for more realistic models to represent the plastic behavior of complex polymeric structures [19].

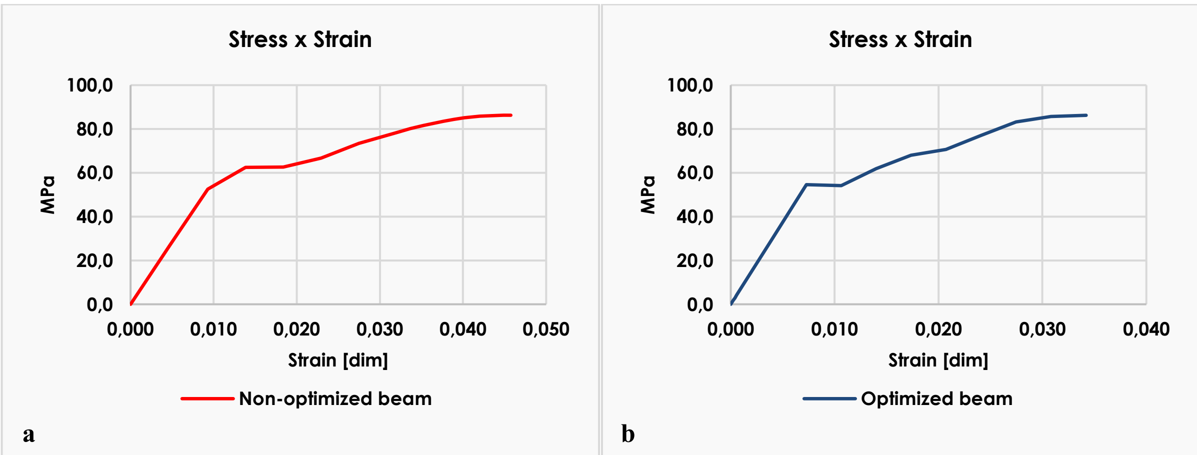

Figure 8 – Von Mises stress vs. strain. (a) Non-optimized beam; (b) Optimized beam.

4 Conclusions

This study presented and validated a computational–experimental workflow for the development of polymeric components optimized through additive manufacturing. The methodology integrated topology optimization using the SIMP method, the application of diamond-type lattice structures, and fabrication via FDM, resulting in a PLA beam with mechanical properties tailored to the structural loading.

The discrepancies between simulated and experimental results, especially in the plastic region, arise from a combination of physical factors related to the FDM manufacturing process and the simplifications assumed in the numerical model. The most relevant factor is the anisotropy of printed PLA. The FEM model assumes the material to be isotropic, with uniform properties in all directions, whereas FDM-fabricated parts exhibit orthotropic behavior [8]. The interfaces between layers and filaments constitute weak zones that are not adequately represented in the simulation, leading to overestimation of strength and stiffness.

Another important aspect is the presence of manufacturing defects such as micro-voids and discontinuities, which reduce the effective load-bearing area and act as stress concentrators. Such imperfections are particularly critical at the junctions of the lattice struts, where failure tends to initiate [17]. The geometric idealization adopted in simulation ignores these local defects. In addition, dimensional variations caused by shrinkage or over-extrusion affect the geometric accuracy of the actual part relative to the CAD model, impacting the observed mechanical response.

Topology optimization, by concentrating material in regions of higher demand, increases structural stiffness but compromises the capacity for plastic deformation. As a result, the optimized beam exhibits brittle behavior, unlike the solid beam, which retains ductility. This change in failure mode imposes constraints on the use of topology-optimized designs in applications where energy absorption is critical, underscoring the need for alignment between the design criterion and the expected structural behavior [19].

In summary, the present work provides a robust validation of a topology optimization approach applied to additive manufacturing, highlighting its benefits, limitations, and potential for technological development.

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Authorship statement. The authors hereby confirm that they are the sole liable people responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property of the authors or has the permission of the owners to be included here.

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