

# Thermomechanical Modelling and Shape Prediction in 4D Printing Using FEA

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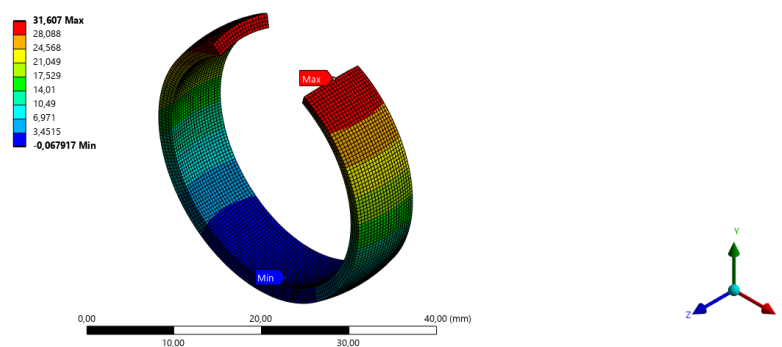
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**Abstract.** In today's competitive manufacturing landscape, balancing cost and performance is crucial. Additive Manufacturing (AM) offers a path to efficient, functional designs, with Four-Dimensional (4D) printing emerging as a key innovation. By using materials that are responsive to external stimuli, 4D printing enables objects to change shape over time, making them active and opening new possibilities in adaptive design. Building on this, research into the shape morphing behaviour of 4D-printed objects was conducted through simulation. Based on the literature, this process can be effectively approached as a thermomechanical problem. This work first simulates the shape morphing of two-layer structures. Multiple parameters are varied through Finite Element Analysis (FEA) to assess both their independent influence and the feasibility of the proposed method. The study then analysed the use of orthotropic properties to evaluate control over deformation directions. Finally, insights from these phases were applied to more complex geometries. It is concluded that the morphing process can be computationally planned using a thermomechanical approximation, paving the way for the incorporation of the influence of printing parameters, pattern design and the strategic division into active/passive regions. This study provides foundational work in 4D printing regarding the shape prediction of printed objects.

## Introduction

Modern manufacturing is shaped by the ongoing pursuit of greater efficiency, functionality, and cost-effectiveness. As industries evolve to meet complex design demands, Additive Manufacturing (AM) (commonly referred to as 3D printing) has become a transformative technology. It allows for the direct fabrication of intricate, customized components from digital models, reducing material waste and streamlining production processes. Extending the capabilities of AM, Four-Dimensional (4D) printing introduces the dimension of time by incorporating smart materials that react to external stimuli such as temperature, light or magnetic fields (Figure 1). These responsive materials enable printed objects to dynamically alter their shape, behaviour or function over time, paving the way for innovative, adaptive applications in fields such as aerospace, biomedicine, defence and construction [1–10].



**Fig. 1.** Representation of the morphing process from a variation of the ratio of CTE in a bilayer beam.

Despite the rapid advancement and growing range of applications of 4D printing, one of the main challenges impeding its widespread adoption is the difficulty in predicting and designing the final shape and behaviour of printed parts. Notably, the morphing process involves complex interactions among multiple variables, namely material composition, geometry, stimulus conditions and printing parameters. Accurate prediction models are essential for controlling and programming these transformations effectively remain underdeveloped [11–18].

Recent studies such as Zeng *et al.* [13], Bodaghi *et al.* [14], Peng *et al.* [15], Tholking *et al.* [16] and Song *et al.* [18] have made strides toward addressing this challenge, demonstrating how anisotropic properties can be embedded into a structure via Fused Deposition Modelling (FDM) and other Material Extrusion (MEX) technologies, given its material compatibility, operational accessibility and relevance to the development of 4D printing, enabling controlled deformation under thermal stimuli without post-processing. These approaches demonstrated how anisotropic material properties can be strategically exploited to program deformation directionality under thermal activation. In these cases, emphasis was placed on material orientation and interlayer stiffness mismatches in order to induce shape morphing behaviour.

Remarkably, several works [8,11,16,19–25] demonstrated that 4D morphing can be effectively simulated using thermomechanical models, where mismatches in properties such as the coefficient of thermal expansion (CTE) and Young's modulus drive shape transformation. These works underscore the relevance of simulating 4D printing behaviour as a thermomechanical problem, particularly for bilayer structures, and highlight the potential of tailoring deformation by adjusting parameters such as material orientation, activation temperature, and dimensions. Nevertheless, it can be noted that previous contributions remain mostly application-specific, often relying on experimental calibration or narrowly scoped simulations. There is a need for a generalisable, computationally efficient modelling framework that captures the essential mechanics of 4D shape transformation, particularly relevant during the early stages of design, where physical prototyping may not be feasible. Moreover, existing works don't often explore the programming potential of orthotropic properties in simulation environments, despite their practical relevance in FDM-based 4D printing.

The present work aims to contribute to shape prediction strategies in 4D printing through a computational approach. In this case, the main objective is to develop and validate a numerical simulation models based on Finite Element Method (FEM) that accurately represent the shape-morphing behaviour of 4D-printed objects under thermal activation. The study begins with simple bilayer configurations to isolate and examine the influence of key parameters, then advances toward complex geometries incorporating directional control and strategic material distribution. By analysing these effects in a controlled digital environment, this work provides a conceptual framework for guiding the design and programming of 4D-printed systems.

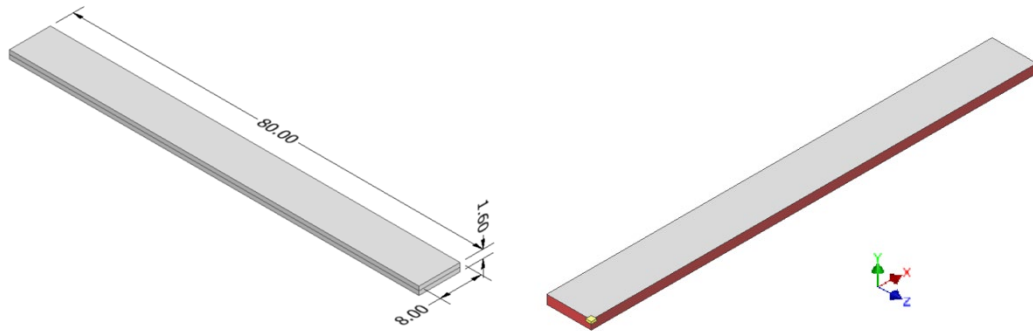
A key aspect of the adopted strategy is its exploratory and conceptual nature. Rather than replicating every physical detail of the printing process, the method explored the potential of a simplified approach to the problem by modelling 4D shape change as a purely thermomechanical phenomenon, following literature guidelines. This treats deformation as the result of internal stress imbalances generated by mismatches in thermal expansion and stiffness between material regions when subjected to a uniform thermal load. Although this approach does not fully capture time-dependent effects or complex multi-physics interactions, it offers an effective approximation for studying and programming shape transformation. This balance between apparent simplicity and predictive power contributes to a systematic framework for shape prediction, offering researchers a scalable tool to guide the development of programmable, stimuli-responsive systems in 4D printing.

### **Thermal stimuli simulation**

An initial analysis investigates the thermomechanical behaviour of 4D-printed bilayer structures under thermal stimuli, aiming to clarify how key material and geometric parameters govern shape morphing. A simulation-based approach using FEA was adopted, treating morphing as a mechanically driven deformation problem induced by uniform heating. Controlled parametric studies

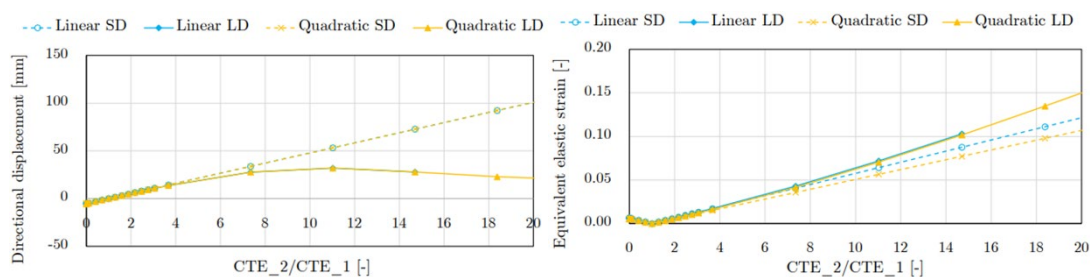
were conducted to assess how variations in the CTE, Young's modulus, activation temperature, thickness, and length influence the structure's response.

The reference model was a bilayer beam,  $80 \times 8 \times 1.6$  mm, with bonded layers (Figure 2). The top layer remained fixed as Poly(lactic acid) (PLA), while the bottom layer's properties were varied to study their effects – such as the CTE, Young's modulus, activation temperature, layer thickness and beam length. A thermal variation of  $125^\circ\text{C}$  was applied to activate the system and a minimal constraint method was applied to allow free thermomechanical deformation (Figure 3). To assess solver behaviour and geometric nonlinearity, four numerical formulations were compared: linear and quadratic elements under both small and large deflection assumptions.



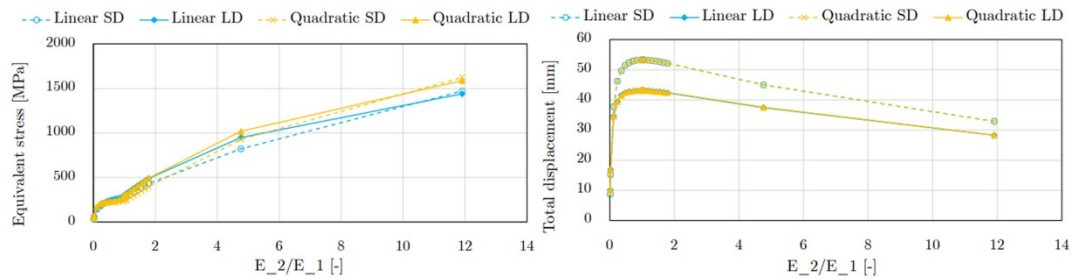
**Fig. 2.** 3D representation of the used geometry and the constraints applied to the model.

CTE emerged as a dominant driver of morphing abilities. The layer with the higher CTE consistently dictated the bending direction, with the structure curling away from it due to thermal strain mismatch. As the CTE ratio increased, curvature intensified, though nonlinearly. When only one material's CTE was altered, low values yielded minimal deformation, revealing an asymmetry in behaviour. In fact, it was noted that at very low CTE values, the ability of that layer to contribute to deformation diminished, nullifying its morphing role. These trends aligned with thermomechanical theory, where expansion produces internal moments that induce curvature. Notably, the small deflection solver failed to capture the expected curling, producing unrealistic stretching due to its static stiffness assumption. In contrast, the large deflection solver accurately represented the geometry and stress redistribution during deformation. This validated the need for nonlinear formulations when simulating thermally driven shape changes. The results from the CTE influence are presented in Figure 3.



**Fig. 3.** Data acquired from the CTE study: displacement in the Y direction (left) and elastic strain (right).

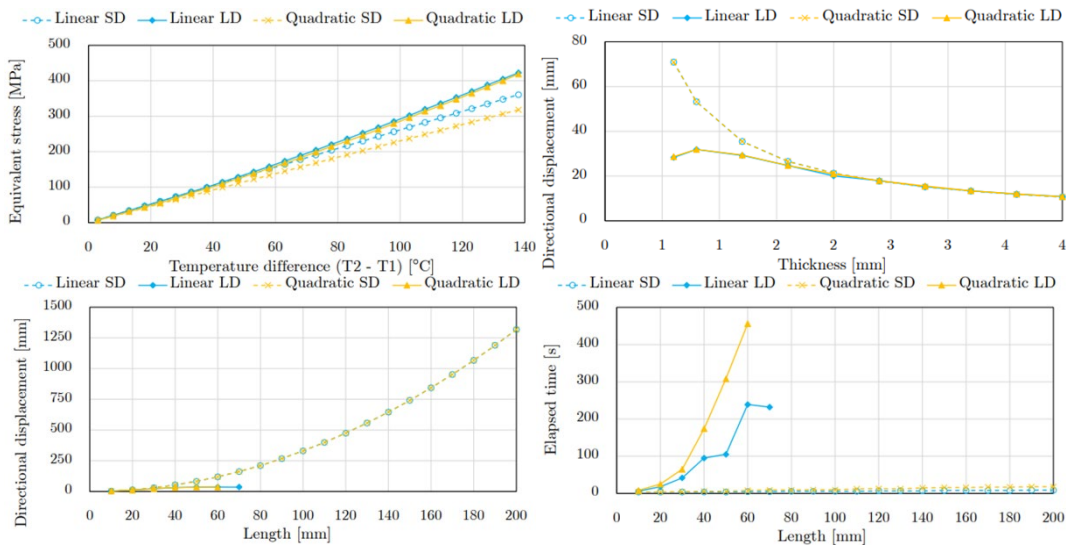
The role of Young's modulus showed a complementary yet distinct effect. Maximum displacement occurred when both layers had similar stiffness, allowing cooperative bending. As the modulus ratio increased, deformation decreased and internal stress rose, where energy was stored instead of released via curvature. These results reinforced that thermal and mechanical strains act together, and that higher stiffness limits deformation while amplifying stress. Again, nonlinear solvers were necessary to correctly capture these interactions under large deformations. Figure 4 presents the obtained results from the Young's modulus variation.



**Fig. 4.** Results attained from the Young's modulus study: equivalent stress (left) and total displacement (right).

Together, CTE and Young's modulus studies revealed that bilayer deformation can be precisely guided by tuning either thermal expansion or stiffness. The direction and degree of morphing are dominated by the CTE ratio, while the modulus ratio influences the balance between deformation and stress. This justifies a modelling focus on one of these two parameters for predictive and controllable design in a computational environment.

Further studies explored geometric influences. Higher activation temperatures increased deformation, particularly under nonlinear solvers, confirming the link between thermal input and strain. Increasing thickness reduced displacement, as expected from bending theory, but internal stress profiles remained relatively unchanged, highlighting continued mechanical response. Length scaling showed greater deformation with size, though nonlinear effects again necessitated large deflection solvers. At larger scales, convergence difficulties emerged, pointing to computational limits in simulating extensive morphing. Figure 5 further illustrates these remaining studies.



**Fig. 5.** Data acquired from the remaining studies: (a) equivalent stress, (b, c) directional displacement, (d) simulation time.

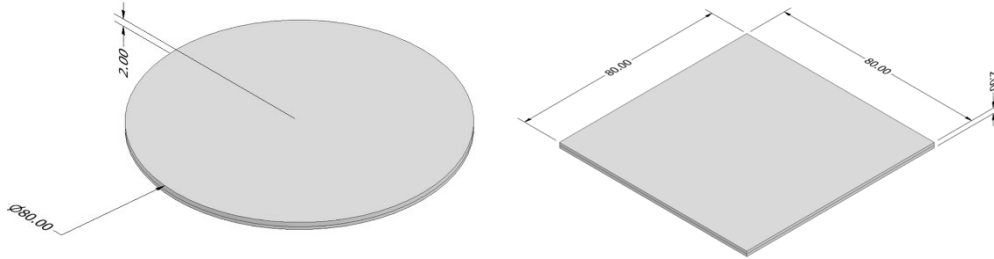
In summary, this phase established a clear methodology for simulating thermomechanical shape change in bilayer structures. It confirmed that nonlinear geometric formulations are essential, and that CTE and Young's modulus are the most effective levers for design control. These insights provide a foundation for more complex morphing simulations in later development stages.

### Orthotropic properties evaluation

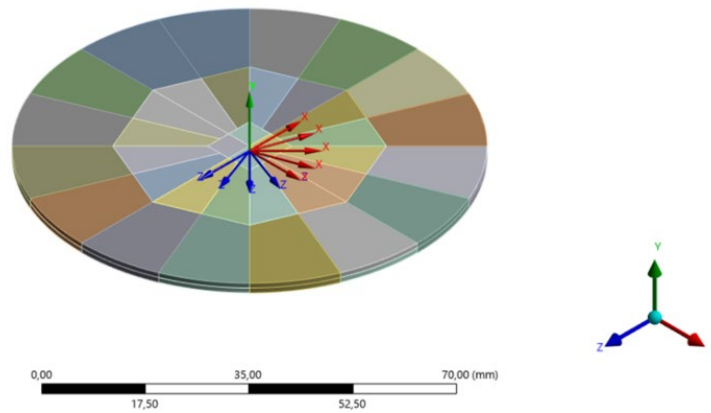
To assess directional control in 4D-printed structures, a second phase of simulations was carried out using orthotropic material properties, representing a more realistic approximation of printed parts. Two geometries, a cylindrical model and a square model (Figure 6), were analysed to evaluate how anisotropic thermal expansion affects deformation behaviour under thermal loading. Both retained the PLA top layer while the bottom layer's material was assigned orthotropic properties with varying

principal directions (Figure 7). This allowed the simulation of directionally dependent expansion akin to that observed in printed filament paths.

A sequential methodology of five parametric studies per geometry was employed: initial studies replicated the isotropic behaviour for comparison, followed by cases varying directional CTEs along specific axes, and culminating with a sweep of orientation angles to map out morphing directionality.



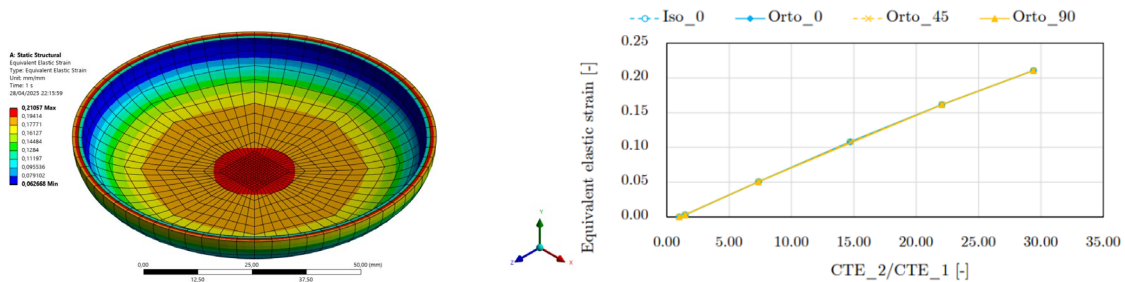
**Fig. 6.** 3D illustration of the analysed geometries.



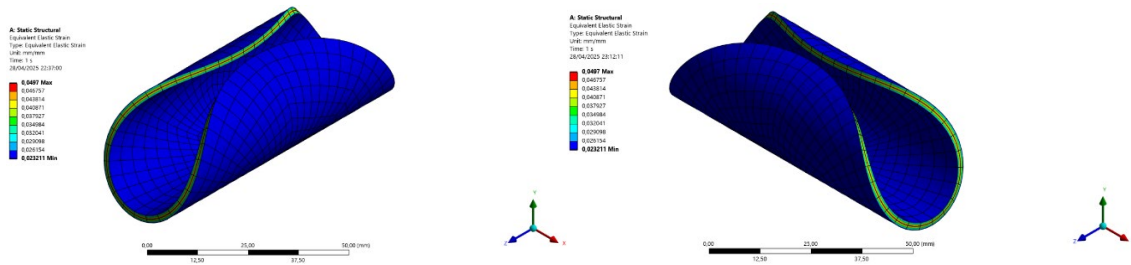
**Fig. 7.** 3D representation of the assignment of different material directions.

Results from the cylindrical model showed radially uniform deformation, confirming that, under uniform geometry and symmetric boundary conditions, shape morphing direction is unaffected by orthotropic property assignment when expansion is equal in all directions (Figures 8 and 9). Conversely, in the square model, the presence of geometric asymmetries led to highly directional deformation patterns. Varying the orientation of the orthotropic properties caused a shift in the morphing direction, with corners exhibiting amplified deformation due to their structural isolation (Figure 10).

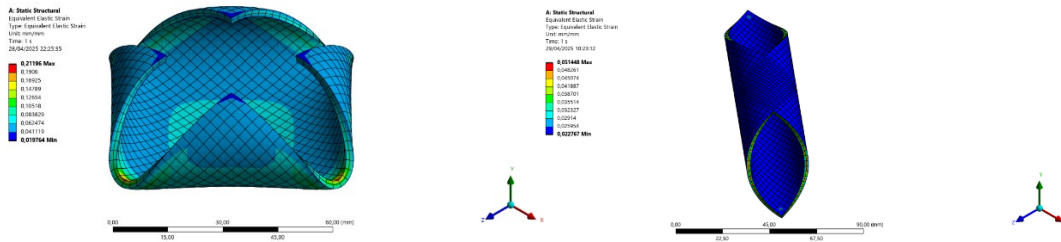
These findings confirm that directional material assignment effectively controls the orientation of shape morphing without significantly affecting stress, strain, or displacement magnitudes, provided that the material distribution remains uniform. Together with previous results, this underscores that the deformation direction in 4D-printed bilayers can be governed by both the CTE ratio between layers and the spatial orientation of material properties, enabling tailored actuation through anisotropic design.



**Fig. 8.** Equivalent elastic strain data from a cylindrical model: 3D results for an isotropic model (left); data acquired from an isotropic model and orthotropic models for validation.



**Fig. 9.** Results achieved by the cylindrical model, varying the bottom body's CTE in only one direction, with a principal material direction in the X axis (left) and Z axis (right).

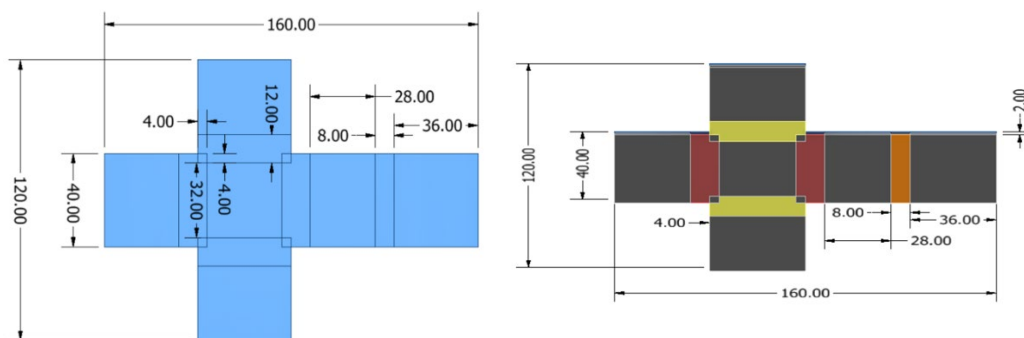


**Fig. 10.** Results obtained from the square model analysis: isotropic model (left) and orthotropic model (right).

### Shape prediction tests

Building on previous results that highlighted the influence of key parameters, such as Young's modulus and CTE ratio between layers, structural dimensions, material orientation, and stimulation temperature, an integrated computational methodology was developed to predict 2D-to-3D shape transformations.

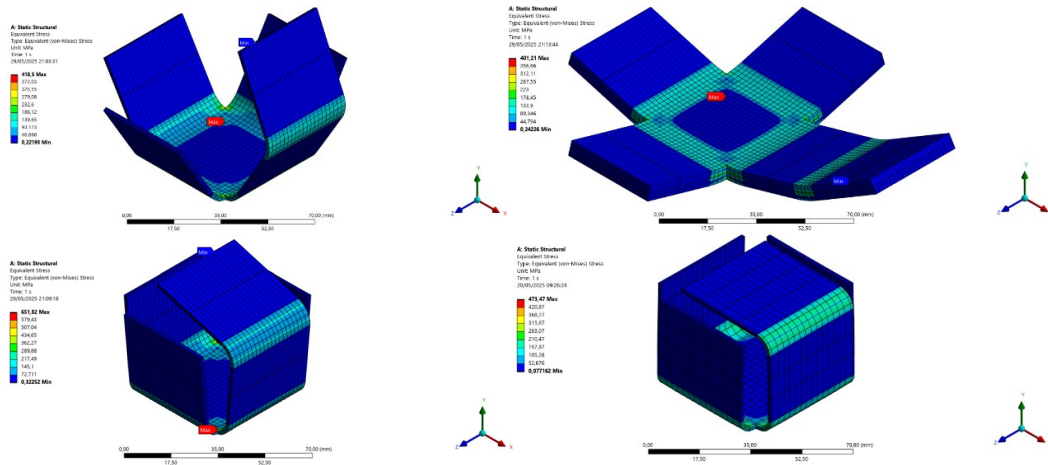
The strategy began with the design of a 2D two-layer pattern programmed to morph into a cube, selected for its straightforward uniaxial deformation behaviour and its suitability as a benchmark. Inspired by origami principles, the model featured hinge-like active regions at the edges and passive regions on the faces. Material properties were strategically assigned: the top layer remained passive, while the bottom layer included directional active segments ( $0^\circ$  or  $90^\circ$ ), driving localized bending at critical edges. Figure 11 further illustrates this methodology. The cube's faces were modelled as individual bodies with bonded contacts and minimal constraints to enable free deformation. Uniform thermal loads triggered the transformation, and a series of calibrations explored how stimulation temperature, CTE ratios, structural thickness, and critical region length influenced the outcome.



**Fig. 11.** 3D illustration of the cube model, representing the division in multiple regions.

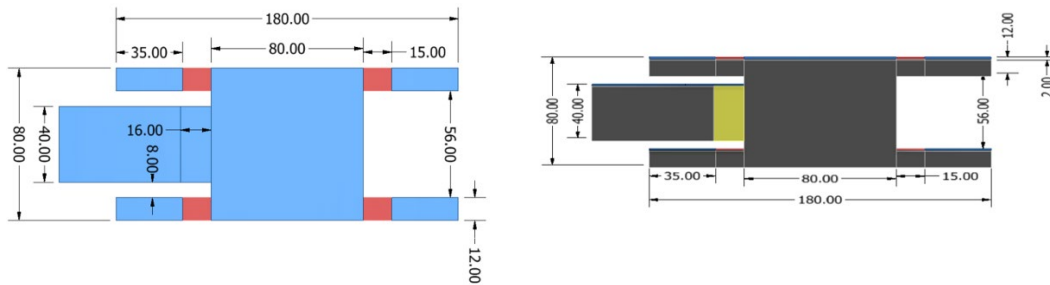
The initial tests revealed that increasing stimulation temperature or CTE ratios enhanced deformation but led to unfeasibly high stresses, especially near face junctions, questioning their real-world applicability. Subsequent calibrations refined the morphing behavior by introducing independent control over the top face, and by adjusting the offsets of active regions from shared vertices, reducing stress concentrations. A final set of tests shifted lateral edge starting points to tune morphing symmetry. Figure 12 provides a better understanding of the obtained results. Overall,

results showed that complex shape programming requires not only correct directional assignment and CTE control, but also geometric tuning to mitigate mechanical incompatibilities.

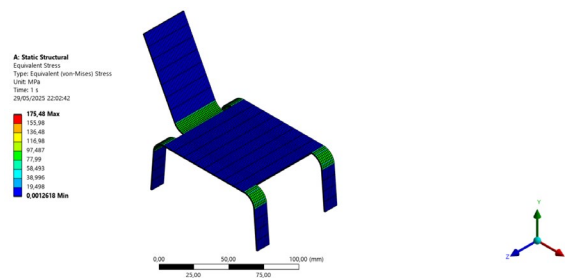


**Fig. 12.** Exemplification of the cube's morphing process.

After validating the methodology with the cube, the approach was applied to more complex geometries to demonstrate its versatility. A chair-like model explored multi-axial deformation, with active regions placed at the leg-seat and seat-back interfaces (Figures 13 and 14). Programming material activity layer-wise induced downward leg folding and upward backrest motion. Calibration showed that the degree of morphing was primarily influenced by the length of active regions along the deformation axis, with negligible sensitivity in the perpendicular direction.



**Fig. 13.** 3D illustration of the chair model, representing the division in multiple regions.



**Fig. 14.** Illustration of the chair's morphing process.

A flower model introduced opposing petal deformations, requiring more intricate material orientations ( $0^\circ$ ,  $45^\circ$ ,  $90^\circ$ ,  $135^\circ$ ) and active region control. Though geometrically more complex, the same core methodology enabled differentiated petal movements, validating the directional and regional assignment strategy, as it can be seen in Figures 15 and 16.

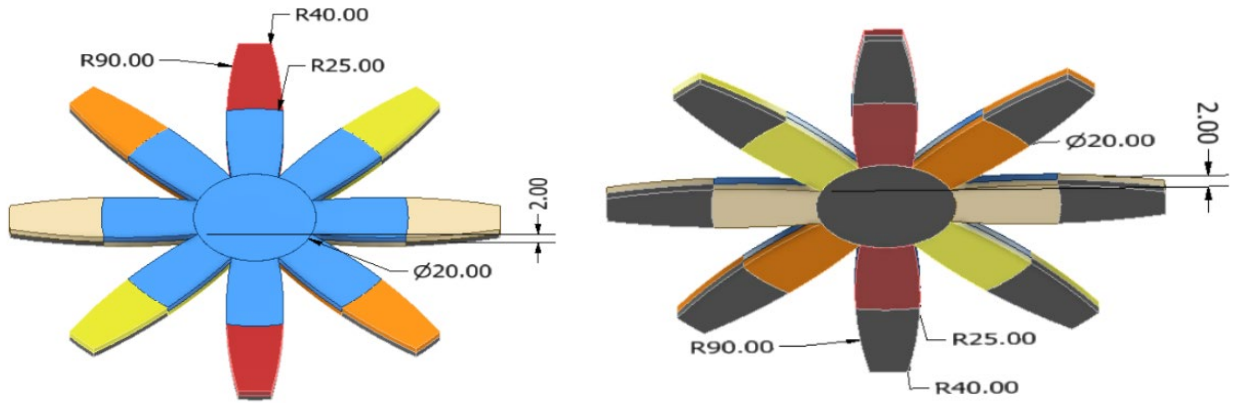


Fig. 15. 3D illustration of the flower model, representing the division in multiple regions.

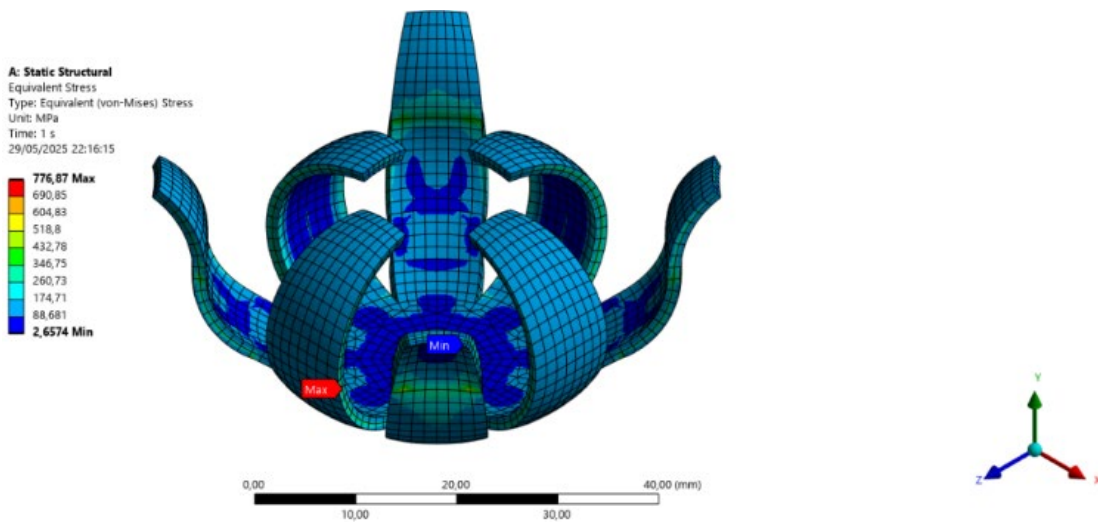


Fig. 16. Exemplification of the flower's morphing process.

Finally, a serpent-inspired model incorporated torsional behaviour. Its segmented body used alternating material orientations and layer dominance to generate slithering motion, while the head and hood were independently programmed. A four-step calibration confirmed that torsion, bending, and complex sequencing could be achieved through controlled parameter variation, again reinforcing the modular and scalable nature of the computational strategy. Figures 17 and 18 further illustrates the obtained results.

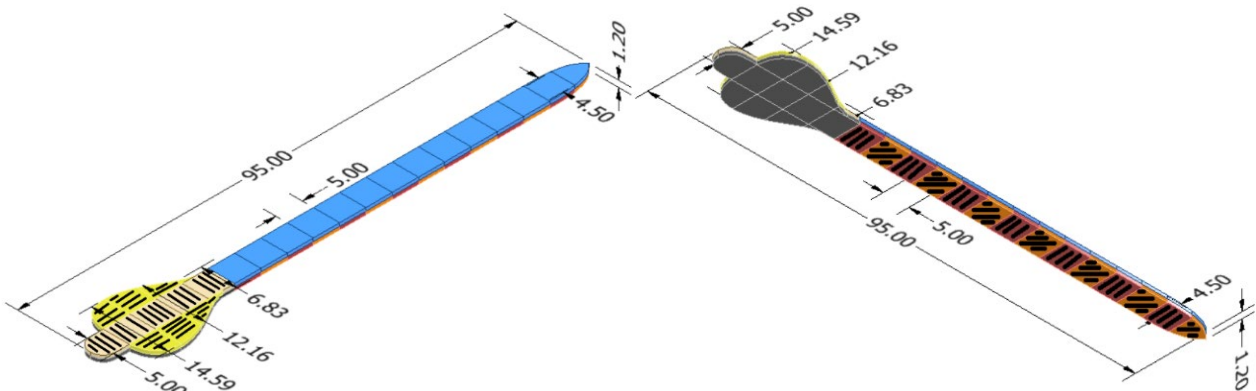
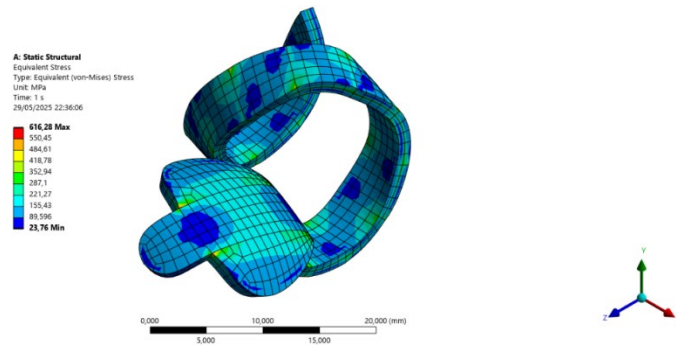


Fig. 17. 3D illustration of the snake model, representing the division in multiple regions.



**Fig. 18.** Exemplification of the snake model's morphing process.

This sequence of models, increasing in complexity, demonstrated that programmable deformation can be achieved through careful region subdivision, strategic material orientation, and layered property assignment. While real-world implementation still requires refinement, particularly regarding the physical definition of active/passive regions, the results offer a structured path toward predictive shape control in 4D printed systems.

## Conclusion

This work presented a simulation-based methodology for predicting shape morphing behaviour in temperature-responsive 4D-printed structures. By treating the process as a thermomechanical deformation problem, it was possible to evaluate the impact of key design parameters, including CTE, Young's modulus, activation temperature, thickness, and geometry, on the performance of bilayer systems. Finite Element Analysis showed that shape transformation can be effectively controlled by tuning either thermal expansion or stiffness, with CTE emerging as the dominant factor in defining deformation direction.

The methodology was further extended using orthotropic properties to program deformation orientation, confirming that directional control can be achieved through anisotropic material assignment. This was validated in increasingly complex geometries, where programmable segmentation enabled the prediction of 3D shapes from 2D patterns.

Notably, this research contributes a flexible and scalable numerical strategy for the design of adaptive 4D-printed components. Future developments should focus on improving the definition of active and passive regions in printed structures, further incorporating variable printing parameters, such as speed, pattern, and thickness, into the simulation environment. Nevertheless, an experimental component would be crucial for a proper validation of this research field. Overall, these refinements would help close the gap between digital prediction and physical performance, supporting more accurate and reliable shape programming in practical applications.

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## Declaration of Generative AI and AI-Assisted Technologies in the Writing Process

The authors acknowledge the use of ChatGPT (OpenAI, <https://chat.openai.com>) as a copilot for brainstorming topics related to this work and for assisting with English language corrections, particularly in identifying improvements in writing style.

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