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Graphical Abstract

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Highlights

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- A novel cellular modeling method blending function representation with skeletal graphs for enhanced design flexibility.
- Seamless topology transitions in cellular structures for complex design adaptability.
- Utilizes open-source tools for advanced cellular structure generation, setting a foundation for future innovation.

Geometric modeling of advanced cellular structures with skeletal graphs

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Abstract

This paper introduces an approach for the geometric modeling of advanced cellular structures, characterized by their stochastic, conformal nature, and the ability to transition between multiple topologies. Utilizing a function representation-enhanced topological skeletal graph methodology, this approach enhances computer-aided design by encapsulating complex geometries and parameters within a versatile function representation framework. The novelty of this work lies in its operationalization through LatticeQuery, an open-source software, which demonstrates versatility in modeling stochastic cellular structures, ensures smooth topology transitions, and supports the design of conformal cellular structures. This exploration not only validates the potential of the introduced methodology but also opens new avenues in the design of cellular structures with intricate geometries and variable properties, catering to a wide range of industrial applications.

Keywords: geometric modeling, computer-aided design, additive manufacturing, computational geometry, function representation, design methods

1. Introduction

The rise of additive manufacturing (AM) techniques has significantly expanded the capabilities of engineering design. Notably, these techniques enable the creation of intricate cellular structures, as illustrated in Fig. 1. These

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structures, ranging from stochastic and conformal to multi-topology surfacebased ones, present unique design challenges [1, 2]. Expanding upon the approach we proposed in our preceding paper, this work carries out an exploration study, focusing on more advanced cellular structures, namely cellular structures that are stochastic, heterogeneous conformal, and heterogeneous surface-based with multiple topologies, given their intricate geometries and unique capabilities.



Figure 1: Advanced cellular structures fabricated using additive manufacturing. (a) A stochastic lattice cube demonstrating random interconnectivity, (b) a dome-shaped conformal lattice with uniform perforations following the surface curvature, and (c) a shoe sole featuring a heterogeneous cellular design, combining different thickness patterns for tailored cushioning and support.

In the realm of AM, the geometric modeling of cellular structures necessitates careful consideration of several key factors to ensure manufacturability and functional integrity. The design of lightweight structures realized via AM, particularly those with cellular configurations, requires an understanding of the process-material property relationship and the integration of non-uniform material design [3]. For instance, Dielemans et al. [4] explored the potential of lightweight concrete extrusion in AM, emphasizing the importance of geometric customization for thermal performance in building components with closed cellular structures. Similarly, Großmann and Mittelstedt [5] focused on the manufacturing challenges and elastic properties of two-dimensional cellular solids in AM, highlighting the significance of structure geometry and material volume in achieving high lightweight degrees. Furthermore, the development of machine learning-derived graded cellular structures, as proposed by Challapalli, Konlan, and Li [6], underscores the need for computationally efficient design strategies that account for AM constraints like support structures and powder removal. These studies collectively illustrate the critical role of geometric considerations in the AM of cellular structures, paving the way for innovative design methodologies that harness the full potential of AM technologies.

Designing advanced cellular structures often requires a holistic approach that integrates geometric modeling, finite element analysis (FEA), and topology optimization [7, 8]. FEA plays a crucial role in this framework, particularly in assessing the load capacity and mechanical properties of the designed structures. By simulating the physical behavior under various loading conditions, FEA provides insights into the structural integrity and performance of cellular structures, guiding the optimization process for enhanced functionality and efficiency [9, 10]. Implicit techniques, such as topology optimization, use mathematical equations to define shapes, facilitating the efficient handling of complex geometries [11, 12]. However, these techniques often yield limited control over the final outcome due to their indirect geometric representation. The integration of FEA with geometric modeling and topology optimization ensures a more comprehensive and accurate design process, allowing for the creation of cellular structures that are not only geometrically complex but also mechanically robust and optimized for specific applications [13].

Conversely, explicit geometric modeling techniques allow for direct manipulation of geometric elements like vertices, edges, and faces [14, 15, 16]. This approach generally manages complex and irregular geometries more effectively and is not reliant on specific mathematical representations [17]. Taking into the account potential drawbacks associated with visual programming language (VPL) interfaces in CAD, such as issues with flexibility, scalability, and user accessibility [18, 19], the focus of this work leans towards explicit modeling. This preference stems from rapid iteration capabilities of explicit modeling, direct manipulation, and effective handling of complex geometries [20]. It is important to note that advancements in explicit modeling often accompany and contribute towards developments in implicit techniques [21, 22].

Stochastic cellular structures exhibit enhanced mechanical properties like energy absorption and impact resistance [23, 24]. Their design, however, presents challenges due to their inherent complexity and variability [24, 25]. Techniques such as Voronoi tessellation and Delaunay triangulation are used for designing these intricate geometries [26, 27].

Recent advancements in the geometric modeling of stochastic cellular structures have significantly enhanced the capabilities of AM [28, 29]. The work by Tang, Dong, and Zhao [30] introduces a hybrid geometric modeling method that integrates various approaches to efficiently and flexibly generate cellular structures tailored for desired properties, a crucial aspect in AM. This method not only simplifies the design process but also ensures that the complex geometries inherent in stochastic structures are manufacturable. Furthermore, the study by Stadlbauer et al. [31] on interactive modeling of stochastic cellular structures on surfaces has opened new avenues in AM. This approach allows for direct modeling and editing of cellular structures on surface meshes, which is particularly beneficial for creating intricate patterns and designs that are often required in stochastic cellular structures. This method, featuring efficient implementation on graphics hardware, aligns well with the needs of modern support-free AM platforms, offering a significant leap in the design and production of complex cellular geometries.

Conformal cellular structures are specifically designed to follow or 'conform' to a pre-defined surface shape. Their design process requires geometric modeling and involves a range of methods, each with its own advantages and drawbacks [1]. Hybrid geometric modeling methods generate tessellated geometric models of cellular structures by optimizing the orientation and size of the struts, thereby improving mechanical properties [32, 30]. However, these methods are computationally demanding and struggle with intricate surface features and irregular geometries [33]. Projection-based methods utilize conformal maps to generate conformal cellular structures on complex surfaces, but they can result in distortions on highly irregular or complex surfaces [34, 35]. Iso-surface extraction creates a mesh template from the object's surface for the cellular structure, facilitating the handling of complex geometries. However, this method is computationally intensive and has difficulties with high-curvature or complex topology surfaces [36, 33]. Lastly, generative design pipelines offer automated modeling, analysis, and inverse design solving of conformal cellular structures through integrated optimization and FEA frameworks [37]. These pipelines, while promising, require substantial computational resources, and the optimization process can be time-consuming [38]. Additionally, the manufacturability of structures may be constrained by the capabilities of the chosen manufacturing technique [38].

Recent advancements in the geometric modeling of conformal cellular structures, particularly in the context of AM, have led to significant progress and challenges [39, 40]. A notable development is the hybrid geometric modeling method presented by Wang, Chen, and Rosen [32], which effectively creates CAD models of large-scale conformal cellular structures. This method addresses the computational and storage complexities associated with modeling large truss structures in CAD systems, a critical aspect in the design and manufacture of conformal truss structures. However, while this approach automates the geometric modeling process efficiently, it may still face challenges in handling the intricate details and variations of conformal structures at a micro-scale level.

Gómez-Ovalle [41] introduced a computational method to generate porous cellular structures conforming to surfaces with complex geometry. This method is significant in integrating cellular structures in engineering applications with complex macro-geometries. However, while it solves the problem of adapting cellular structures to complex surfaces, the impact of transformations on mechanical properties needs thorough analysis, especially in applications where structural integrity is paramount.

Another advancement is the generative design of conformal cubic periodic cellular structures using a surrogate model-based optimization scheme by Wang and Rai [37]. This pipeline offers automated modeling, analysis, and inverse design solving of cellular structures through integrated optimization and FEA. This method is particularly promising for designing lightweight and high-strength functional parts. However, the reliance on surrogate models may introduce challenges in accurately capturing the nuanced behaviors of complex cellular structures, especially when subjected to real-world loading conditions. Nevertheless, as generative models integrate into more and more aspects of engineering design, it is crucial to provide these models with geometric modeling tools they can operate [42].

Multi-topology surface-based cellular structures embody a unique blend of challenges and opportunities in the realm of geometric modeling [43]. With cubic unit cells, beam-based cellular structures facilitate relatively straightforward topology transitions [44]. However, ensuring defect-free structures in surface-based cellular structures demands smooth topology transitions, a requirement often overlooked in current homogenized models, potentially impacting their mechanical properties [45]. Optimizing these transitions remains a daunting task due to computation times and model defects. Morphing and blending techniques enable smooth transitions between different surface types. Methods such as interpolation-based approaches and parametric blending of different minimal surfaces have been proposed. Moreover, multi-objective optimization algorithms have been examined for optimizing mixed surface-based cellular structures. Despite these advancements, the geometric modeling of multi-topology surface-based cellular structures still confronts substantial challenges like handling complex shapes, preventing defects during topology transitions, and developing efficient algorithms for multi-topology transitions. The pressing need for a comprehensive approach that supports seamless topology transitions underlines a promising direction for further exploration in geometric modeling.

Recent advancements in the geometric modeling of cellular structures with multiple types of unit cells have been instrumental in enhancing understanding and capabilities in designing complex geometries [46, 47]. One significant study in this area is by Sarabhai et al. [48], which focuses on the thermal and flow behavior of 3D printed cellular structures. This research explores the design of various structures, including triply periodic minimal surfaces (TPMS) with varying thicknesses and volume fractions, providing valuable insights into the geometric intricacies of these structures. However, while the study advances understanding of the thermal and flow behavior of these structures, it may not fully address the complexities involved in modeling the interactions between different unit cell types, especially when these interactions significantly impact the overall structural integrity and functionality [49].

The study by Kulikov [50] explores the representation of the state of cellular structures in the form of 'phase portraits' of states at discrete moments in time. This approach, which models the structures as dynamic systems, provides a novel way to visualize and control the process of formation and transformation of cellular structures. However, the complexity of accurately modeling phase transitions in cellular structures, especially when dealing with multiple shapes and forms, remains a significant challenge [51].

The work of Yang et al. [52] presents a novel approach in the field of AM, focusing on the design and fabrication of cellular structures inspired by grain boundaries. This study is significant as it explores the potential of using grain boundary concepts to enhance the mechanical properties of cellular structures, which could have wide-ranging applications in various engineering fields. The integration of grain boundary-inspired designs in cellular structures is an innovative approach that could lead to the development of materials with superior strength and durability. However, the scalability of this approach and its adaptability to different materials and manufacturing settings remains an area for further exploration.

The work of Sanders et al. [53] delves into the integration of multiscale design and micro/nanoscale additive manufacturing to achieve free-form, multiscale, biomimetic structures. The concept of continuous multimicrostructure embedding within an optimized macrostructure geometry is a significant step toward achieving more complex and functionally graded materials. However, the study's success hinges on the ability to accurately control and embed microstructures within 3D printer slices, a process that may require further refinement to achieve the desired precision and scalability in practical applications.

Numerous works have explored the application of topology optimization to the phase transition processes in cellular structures [7, 8]. However, a topology optimization problem is often tuned for a single loading condition. While there are works that adapt topology optimization to multiple loading conditions, they can become computationally intense [54, 55]. Instead, this work mainly focuses on smooth and fast phase transitions that can find applications in conceptual design stages. The speed of geometric modeling is believed to play a major role in concurrent design processes.

Commercial software solutions significantly contribute to the geometric modeling of cellular structures, offering a suite of tools for designing, analyzing, and optimizing these structures for various applications. Notably, nTopology [56] specializes in designing advanced materials and structures, including stochastic and conformal cellular structures. While it possesses robust tools and graphics processing unit (GPU) acceleration for expediting model previews, mesh generation could be time-consuming, a common bottleneck in many CAD software packages dealing with cellular structures.

However, complete control over conformality and multi-topology remains elusive in nTopology and similar software, potentially leading to geometric artifacts – unwanted features or irregularities that may impede the final product's performance, manufacturability, and aesthetics [37, 57]. To mitigate these, advanced geometric modeling techniques such as explicit methods may be necessary, offering better control over conformality and multitopology transitions.

Another prominent CAD software, Autodesk Netfabb [58], focuses on AM, offering a comprehensive suite of tools for designing, optimizing, and preparing 3D printed parts. Although robust in regular cellular design, its capabilities are less extensive when it comes to designing stochastic structures and managing smooth transitions between multiple topologies, posing challenges with complex multi-topology cellular structures [59, 33].

Rhinoceros 3D [60], with its powerful parametric design capabilities and Grasshopper [61] plugin, is a versatile CAD software that enables efficient generation and exploration of conformal cellular structures [62]. However, these software solutions still fall short in providing an interface for modifying cellular structure parameters other than thickness, limiting design freedom [63, 44].

While geometric modeling is extensively employed in designing cellular structures, including stochastic, conformal, and multi-topology surface-based structures, research gaps persist. The need for advanced explicit geometric modeling methods that can integrate with implicit methods such as topology optimization for enhanced user control is apparent. The challenge of designing multi-topology surface-based cellular structures with smooth transitions between different surface-based topologies is particularly pronounced in the context of complex bio-inspired and heterogeneous structures [20]. Addressing the trade-offs between design quality and performance, ensuring manufacturing feasibility, and incorporating multi-scale modeling and machine learning techniques for efficient optimization, remain areas where further research is warranted to advance the geometric modeling of cellular structures [32, 64]. Interested readers are encouraged to refer to our previous works for a more detailed review on existing geometric modeling methods, software packages, and Grasshopper plugins [2, 63].

The rest of this paper is structured as follows. In Section 2, an exploratory study that covers various aspects of geometric modeling is presented, including stochastic cellular structures (Section 2.2), conformal cellular structures with a focus on surface (Section 2.3.1) and volume conformality (Section 2.3.2), and heterogeneous cellular structures with multiple surface-based topologies (Section 2.4). Section 3 delves into the practical implementation of these methods, discussing the intricacies of modeling stochastic (Section 3.1) and conformal cellular structures (Sections 3.2.1 and 3.2.2), as well as the challenges in transitioning between different surface-based topologies (Section 3.3). The paper concludes with Section 4, summarizing the findings and their implications for the field of geometric modeling of cellular structures.

2. Exploratory study of function representation with skeletal graphs for the geometric modeling of advanced cellular structures

This section embarks on an exploratory journey into F-rep enhanced with skeletal graphs for geometric modeling of advanced cellular structures. We extend and refine our prior framework [63] to encompass a broader spectrum of cellular structures, including stochastic, conformal, and surface-based topologies with multiple topologies. This enhancement is a response to the growing need for more versatile and intricate design capabilities in geometric modeling, particularly in AM [65]. This approach leverages skeletal graphs, which serve as a backbone for representing the connectivity and structural integrity of these complex cellular forms [66]. The section is organized into several focused subsections, each addressing a specific aspect of this advanced modeling technique.

Multiple software implementations have been developed for modeling cellular structures, each offering unique features and capabilities. For instance, the work by Moj et al. [67] focuses on developing workflows for designing strength test specimens using DMLS/SLM and SLS technologies. This approach emphasizes the importance of obtaining a real solid model of the specimens, showcasing the software's capability in handling both the design and manufacturing aspects of cellular structures Furthermore, Liu et al. [68] introduced a novel rectangular-circular grid-filling pattern for fused deposition modeling in cellular structures. This development highlights the ongoing innovation in software implementations for additive manufacturing, catering to the specific needs of cellular structure fabrication. A more detailed review of existing software implementations is available in our preceding works [2, 63].

Subsection 2.1 delves into the use of F-rep in modeling heterogeneous cellular structures, highlighting how this method can be augmented through skeletal graphs. Subsection 2.2 explores the geometric modeling of stochastic cellular structures, demonstrating the application of the proposed method in creating random yet structurally coherent designs. The study then transitions to the modeling of conformal cellular structures in Subsection 2.3, with a particular emphasis on surface (Subsection 2.3.1) and volume conformality (Subsection 2.3.2), thereby addressing the challenges of adhering cellular structures to predefined shapes. Finally, Subsection 2.4 investigates the geometric modeling of heterogeneous cellular structures with multiple surface-based topologies, showcasing the capability of the proposed approach to handle complex transitions between different topologies. This structured exploration aims to provide comprehensive insights into the capabilities and versatility of F-rep combined with skeletal graphs, paving the way for innovative applications in geometric modeling.

2.1. Function representation in geometric modeling of heterogeneous cellular structures enhanced with skeletal graphs

Function representation (F-rep) is a robust technique for solid object representation in geometric modeling, excelling at defining and manipulating complex 3D cellular structures [69]. Recent advancements in F-rep have focused on enhancing its capability to model materials with varying density and mechanical properties, particularly useful in the context of functionally graded materials (FGMs) [70].

In F-rep, a solid body is characterized by the function $F(\mathbf{X})$ such that

$$F(\mathbf{X}) \ge 0,\tag{1}$$

where $\mathbf{X} \subset \mathbb{R}^3$ is the design space [11]. To incorporate material heterogeneity, the function can be augmented by a density distribution function $D(\mathbf{X})$, yielding a new representation $F_H(\mathbf{X}) = F(\mathbf{X}) \cdot D(\mathbf{X})$.

F is defined so that $\mathbb{S} = {\mathbf{X} | F(\mathbf{X}) \ge 0}$ represents the solid body and $\overline{\mathbb{S}} = {\mathbf{X} | F(\mathbf{X} < 0)}$ is the remaining design space, with $\partial \mathbb{S} = {\mathbf{X} | F(\mathbf{X}) = 0}$ as the solid body boundary.

F-rep can be used for the geometric modeling of procedural functionbased spatial microstructures, which highlights the ability of F-rep to model heterogeneous objects containing internal spatial geometric structures [69]. This approach is particularly useful for creating detailed models of cellular microstructures, as well as irregular porous media. The compact and precise nature of these models, which can undergo various geometric operations, underscores the adaptability of F-rep in handling complex geometries.

Kartasheva et al. [71] delve into the modeling and rendering of heterogeneous objects using implicit complexes within a cellular-functional framework. This work demonstrates how F-rep can be effectively combined with cellular representations to create hybrid models that capture the intricacies of various dimensional entities within a single framework.

However, a review of the existing literature reveals certain challenges. While F-rep provides a powerful tool for modeling complex structures, the computational intensity required for rendering and fabricating these models can be significant [72]. Moreover, the integration of F-rep with other modeling techniques, such as skeletal graphs, to enhance its capability in representing complex topologies is an area that requires further exploration [73].

Despite the challenges related to computational efficiency and the integration with other modeling techniques, F-rep stands out as a promising approach in the geometric modeling of heterogeneous cellular structures, offering precision, versatility, and the ability to handle complex geometries.

Our previous work [63] proposed a framework for the geometric modeling of heterogeneous cellular structures using F-rep enhanced with skeletal graphs. The framework extends the original F-rep model in Equation 1 to

$$F(\mathbf{X}) = (P \circ T)(\mathbf{X}) \ge 0, \tag{2}$$

where $P(\mathbf{X})$ defines geometric parameters distribution, and $T(\mathbf{X})$ defines the cellular structure topology using skeletal graphs. The function $T(\mathbf{X})$, in particular, is enhanced to include adaptive topology control, allowing for the optimization of structural performance under varying load conditions [44].

To model the variation in parameters such as truncation t(z) and thickness h(z) along a particular axis (the z-axis, in this case), the function P can be refined to:

$$P(\mathbf{X}) = G(t(z), h(z)), \tag{3}$$

where G is a functional interaction between t(z) and h(z), and it may represent any composite behavior as needed for the specific application or geometric representation.

The proposed approach supports a higher variety of geometries compared to other existing solutions like nTopology [56] by supporting non-linear functionally graded geometric parameters and incorporating skeletal graphs for topology representation. Skeletal graphs are defined in this work as nodesconnected lines for beam-based cellular structures. For example, a facecentered cubic (FCC) topology can be defined by 12 line segments as

$$T(\mathbf{X}): \begin{cases} \forall i \in \{1, 2, 3\}, & x_i \in \{0, u\}, \\ \forall j, k \in \{1, 2, 3\} \setminus \{i\}, & x_j \in [0, u], \\ x_k = x_j \cdot \delta_{jk} + (u - x_j) \cdot (1 - \delta_{jk}), \end{cases}$$
(4)

where u is the side of the cubic unit cell, δ_{jk} is the Kronecker delta, and x_i, x_j, x_k correspond to x, y, z. The skeletal graph of FCC is depicted in Fig. 2(d). Moreover, parameters such as truncation and cross-section shape can vary, as illustrated in Figures 2(a-c).

The proposed approach also supports heterogeneous conformal cellular structures, exemplified by the tire conceptual design in Figures 3(a) and 3(b), where the cellular structure thickness varies in the radial direction.

2.2. An exploration study of the geometric modeling of stochastic cellular structures using function representation and skeletal graphs

This paper introduces a novel advancement in the original method of modeling beam-based cellular structures, tailoring it to more intricately fit



Figure 2: Solid models of cellular structures modeled with LatticeQuery: (a) a Schwarz 'primitive' cellular structure with thickness varying along the z-axis; (b) a truncated cube cellular structure with thickness varying along the y-axis and truncation varying along the z-axis; (c) a face-centered cubic (FCC) cellular structure with thickness varying along the y-axis and beam cross-section transitioning from square to circle along the z-axis [73]. The FCC topology is defined by (d) its skeletal graph.

stochastic scenarios and deftly integrating skeletal graphs to illustrate topology. This advancement incorporates recent developments in computational geometry and stochastic modeling to achieve a more accurate and efficient representation of complex cellular structures [70]. As specified in Equation 2, the topology definition T is paramount. At the outset, T denotes a skeletal graph composed of zero-thickness lines. This graph is delineated within a unit cell. Subsequently, P is applied to establish the geometric properties,



Figure 3: (a) Isometric and (b) profile view of a conformal heterogeneous cellular tire design with beam thickness increasing further away from the wheel axle in the radial direction [63]. LatticeQuery can generate (c) a structure with varying thickness conforming to a surface. (d) The transformation of the design space $\mathcal{N} : \mathbf{X} = (x, y, z) \to \mathbf{X}_{\Phi} = (\xi, \zeta, \eta)$ where \mathbf{X}_{Φ} is Cartesian relative to the surface Φ . The skeletal graph of the cellular structure maintains topology while achieving surface conformality. Here, Φ is considered the middle surface of the cellular structure that fills the volume with thickness h.

such as beam thickness.

To address the challenges posed by stochastic cellular structures, particularly Voronoi tessellations, a modified approach that integrates spatial point processes with graph theory is introduced [74]. In the predecessor model, beam-based unit cells were defined through line segment equations. Nevertheless, certain stochastic cellular structures, namely Voronoi structures, lack a discernible unit cell. As such, T is tasked with defining the skeletal graph for the entire structure.

The generation of Voronoi cellular structures stems from the placement of seeds which, in stochastic scenarios, often adhere to random distributions. Consider a set of seeds $S = \{s_1, s_2, ..., s_n\}$, scattered throughout the design domain **X**. To mathematically model the irregularity and randomness inherent in these structures, a spatial density function $\rho(\mathbf{X})$ can be introduced, which is used to govern the distribution of the seeds S within the design domain \mathbf{X} :

$$\rho(\mathbf{X}) = \frac{1}{\operatorname{Vol}(\mathbf{X})} \sum_{s_i \in S} \delta(\mathbf{X} - s_i),$$
(5)

where δ is the Dirac delta function and Vol(**X**) represents the volume of the design domain. For any point $p \in \mathbf{X}$, its corresponding Voronoi cell, V(p), is given by:

$$V(p) = q \in \mathbf{X} \quad \text{s.t.} \quad \forall s_i \in S, \quad |p - q| \le |s_i - q|.$$
(6)

To further define the relationship between adjacent Voronoi cells, a density correlation function $\kappa(p, s_i)$ is introduced:

$$\kappa(p, s_i) = \rho(p) \cdot \rho(s_i) \cdot |p - s_i|, \tag{7}$$

which quantifies the interaction between seeds based on their proximity and the local density around them.

The boundary between any two adjacent Voronoi cells, V(p) and $V(s_i)$, is the locus of points equidistant to p and s_i . The bisector b_{p,s_i} can be formulated as:

$$b_{p,s_i} = q \in \mathbf{X} \quad \text{s.t.} \quad |p - q| = |s_i - q|. \tag{8}$$

This is realized by visualizing T as a 3D graph structure of interlinked edges at vertices, effectively embodying the skeletal graph. Assume Γ to be a 3D graph consisting of n vertices, denoted as $w_1, ..., w_i, ..., w_j, ..., w_n$, and medges, signified as $\epsilon_{1,2}, ..., \epsilon_{i,j}, ..., \epsilon_{m-1,m}$, ensuring $i \neq j$.

To quantify the randomness or irregularity of the Voronoi tessellation, a stochastic parameter θ can be introduced, defined over the domain based on the distribution of seeds. For a uniformly random distribution, the local variance in the distance between seeds can be taken as an indicator:

$$\theta(\mathbf{X}) = \operatorname{Var}_{\mathbf{X}}(|s_i - si + 1|), \tag{9}$$

where $\operatorname{Var}_{\mathbf{X}}$ is the spatial variance of the distance between adjacent seeds over the design domain.

Consider a random edge $\epsilon_{i,j}$ linking vertices $w_i = (x_i, y_i, z_i)$ and $w_j = (x_j, y_j, z_j)$, as illustrated in Fig. 4(b). Consequently, each edge can be articulated in a parametric form as:

$$\epsilon_{i,j}(\alpha) = w_i + \alpha(w_j - w_i), \tag{10}$$

for $0 \le \alpha \le 1$, or

$$\epsilon_{i,j}(\mathbf{X}): \frac{x-x_i}{x_j} = \frac{y-y_i}{y_j} = \frac{z-z_i}{z_j}.$$
 (11)

An edge $\epsilon_{i,j}(\mathbf{X})$ is considered non-existent, or $\epsilon_{i,j}(\mathbf{X}) = \emptyset$, if vertices w_i and w_j aren't interconnected in Γ or in scenarios where i = j. Here, T is formulated for the composite cellular structure as the union of all its edges:

$$T(\mathbf{X}) = \bigcup_{i=1}^{n} \bigcup_{j=1}^{m} \epsilon_{i,j}(\mathbf{X}).$$
 (12)

Voronoi cellular structures are frequently employed in design for additive manufacturing (DFAM) when a stochastic framework is requisite [75]. In this context, Voronoi tessellation seeds are envisioned to be uniformly dispersed across the design domain \mathbf{X} , adhering to specific distributions like Poisson disk sampling. Distinctively, this study suggests monitoring the edges of a Voronoi cellular structure through a sophisticated edge tracing technique post radial growth from its seeds [76]. The Bézier curve morphs into a straight line by suitably fitting tangent spheres between any trio of adjacent spheres that have Voronoi seeds at their core. Importantly, this algorithm operates at an O(n) complexity [76].

2.3. An exploration study of the geometric modeling of conformal cellular structures using function representation and skeletal graphs

In a novel exploration of the geometric modeling of conformal cellular structures, this subsection underscores the role skeletal graphs assume in achieving topology that seamlessly conforms to designated surfaces or volumes.

This section explores the geometric modeling of conformal cellular structures, utilizing F-rep and skeletal graphs. This approach is aimed at achieving a topology that seamlessly conforms to designated surfaces or volumes, addressing the challenges of modeling complex geometries in a conformal manner. The subsection is divided into two key sections to provide a comprehensive understanding of the methodology. Section 2.3.1 delves into the techniques for tailoring cellular structures to specific surfaces. This involves morphing the design space into an alternate space that maps onto the chosen surface, using skeletal graphs to define the topology of the cellular structure in accordance with surface conformality constraints. Section 2.3.2 focuses on extending these concepts to three-dimensional volumes.



Figure 4: Geometric modeling of stochastic cellular structures. (a) A random graph Γ , (b) an individual edge $\epsilon_{i,j}$ between vertices w_i and w_j of the graph Γ , (c) a mesh of a human femur bone, (d) a stochastic Voronoi infill of this bone, and (e) stochastic Voronoi structures that conform to random polyhedrons.

2.3.1. Surface conformality

This work presents a novel technique for tailoring a cellular structure to a specific surface by morphing the design space \mathbf{X} into an alternate design space \mathbf{X}_{Φ} , which then maps onto a chosen surface Φ . Leveraging skeletal graphs, this study innovatively achieves topology definition of the cellular structure in line with surface conformality constraints.

To ensure a continuous and smooth transformation of the design space, we define a mapping function \mathcal{N} , which maps each point in \mathbf{X} to its corresponding point in \mathbf{X}_{Φ} :

$$\mathcal{N}(\mathbf{X}) = \mathbf{X}_{\Phi} = \Phi(\mathbf{X}),\tag{13}$$

where $\Phi(\mathbf{X})$ is a function that describes the transformation of points from the original design space to the conformal space.

While the transformation $\mathcal{N} : \mathbf{X} \to \mathbf{X}_{\Phi}$ depicted in Fig. 3(d) may not be affine and might not symbolize a vector between points in \mathbb{R}^3 , this is due to the conformal map's grounding in the intrinsic geometry of a surface. Here, the polyhedron edges become geometrically negligible, even as the metric originates from an embedding in \mathbb{R}^3 [77]. By harnessing the skeletal graph representation, the cellular structure embraces the requisite geometric transformations, ensuring surface conformality without sacrificing topology.

To quantify the degree of conformity to the surface, a conformity measure C is introduced:

$$\mathcal{C}(\mathbf{X}_{\Phi}, \Phi) = \int \mathbf{X}_{\Phi} \left| \nabla \Phi - \nabla \mathbf{X}_{\Phi} \right| d\mathbf{X}_{\Phi}, \tag{14}$$

where $\nabla \Phi$ and $\nabla \mathbf{X}_{\Phi}$ are the gradients of the surface and the transformed design space, respectively. This measure helps evaluate how closely the transformed structure adheres to the desired surface.

In this approach, Φ is deemed a middle surface of the cellular structure, and η aligns with the normal unit vector \vec{n}_{Φ} of Φ . Let h denote the thickness of the cellular structure that conforms to the surface Φ . The skeletal graph is used to shape a cellular structure that fits the surface Φ , preserving the thickness h and the intended geometric properties.

To account for local curvature and its impact on the thickness distribution, a curvature compensation function \mathcal{K}_{cs} is introduced:

$$\mathcal{K}_{\rm cs}(\Phi, \vec{n}_{\Phi}, h) = \frac{1}{\kappa_{\rm cs}(\Phi)} \left(h + \delta h(\kappa_{\rm cs}(\Phi)) \right), \tag{15}$$

where $\kappa_{cs}(\Phi)$ is the curvature of the surface at a given point, and $\delta h(\kappa_{cs}(\Phi))$ is the thickness adjustment based on the curvature.

The furthest equidistant surfaces Φ_+ and Φ_- from the middle plane Φ will be placed at h/2 from it in the directions of \vec{n}_{Φ} and $-\vec{n}_{\Phi}$, respectively. Constructing the equidistant surfaces Φ_+ and Φ_- is not always straightforward [78]. If Φ is defined in parametric form $\vec{\Phi}(p,q)$, then the vector \vec{n}_{Φ} can be found as

$$\vec{n}_{\Phi} = \frac{\left(\frac{\partial \vec{\Phi}}{\partial p}(p,q)\right) \times \left(\frac{\partial \vec{\Phi}}{\partial q}(p,q)\right)}{\left|\left(\frac{\partial \vec{\Phi}}{\partial p}(p,q)\right) \times \left(\frac{\partial \vec{\Phi}}{\partial q}(p,q)\right)\right|}.$$
(16)

To enhance the adaptability of the cellular structure to the surface, a local deformation function \mathcal{D} is introduced, which adjusts the shape of the cells based on surface characteristics:

$$\mathcal{D}(\vec{\Phi}, \vec{n}_{\Phi}, \mathbf{X}) = \vec{\Phi} + \lambda(\mathbf{X}) \cdot \vec{n}_{\Phi}, \qquad (17)$$

where $\lambda(\mathbf{X})$ is a deformation parameter that varies across the surface, allowing for a more flexible and precise adaptation to complex surface geometries.

After obtaining \vec{n}_{Φ} , the surfaces Φ_{-} and Φ_{+} can be computed numerically by offsetting every point of Φ by $\pm h\vec{n}_{\Phi}/2$. This numerical approach is assured by obtaining an equation for a line passing along \vec{n}_{Φ} and solving this equation as a system of two equations with the Euclidian distance

$$(x - x_{\Phi})^{2} + (y - y_{\Phi})^{2} + (z - z_{\Phi})^{2} = \left(\frac{h}{2}\right)^{2}, \qquad (18)$$

where $(x_{\Phi}, y_{\Phi}, z_{\Phi})$ is the offsetted point. Additionally, the offset surfaces can be expressed as:

$$\vec{\Phi}_{\pm}(p,q) = \vec{\Phi}(p,q) \pm \frac{h}{2}\vec{n}\Phi(p,q),$$
(19)

where $\vec{\Phi}(p,q)$ is the position vector of a point on the surface Φ parametrized by p and q and $\vec{\Phi}_{\pm}(p,q)$ are the position vectors of the points on the offset surfaces $\vec{\Phi}_{+}(p,q)$ and $\vec{\Phi}_{-}(p,q)$ corresponding to the point $\vec{\Phi}(p,q)$ on Φ .

Note that in general, $(x_{\Phi}, y_{\Phi}, z_{\Phi})$ will have two solutions for $h\vec{n}_{\Phi}/2$ and $-h\vec{n}_{\Phi}/2$. By leveraging the skeletal graph representation, the cellular structure can be effectively conformed to the surface while maintaining the structural topology and achieving surface conformality.

The proposed method for surface conformality using skeletal graphs opens avenues for further research to enhance support for non-Cartesian \mathbf{X}_{Φ} and to consider more complex conformal mapping scenarios. The skeletal graph representation offers a potent and flexible technique for achieving surface conformality while preserving the intricate topological characteristics of the cellular structure.

2.3.2. Volume conformality

While [63] presented a method enabling cellular structures to be conformal to a volume, it lacked support for geometric modeling of cellular structures uniformly filling a designated volume. In this study, a refined approach is introduced, harnessing the skeletal graph representation to safeguard the topology of the cellular structure even as it conforms to a given volume.

To address the challenge of modeling cellular structures conformal to a designated volume, a volumetric mapping function \mathcal{V} is introduced:

$$\mathcal{V}(\mathbf{X}, V) = \mathbf{X}' \in V \mid \mathbf{X} \text{ is transformed to } \mathbf{X}' \text{ within } V, \tag{20}$$

where \mathbf{X}' represents the points in the transformed design space that fill the volume V.

Given a volume V that the cellular structure should uniformly occupy, the skeletal graph $T = (W_T, E_T)$ serves as a crucial blueprint. It guides the structure's connectivity and geometric attributes, ensuring its perfect conformality to the desired volume. Here, W_T signifies the graph's vertices, while E_T denotes the edges connecting the vertices. The skeletal graph can be generally described mathematically as follows:

$$T = (W_T, E_T) = \begin{cases} w_i \in \mathbb{R}^3 \mid i = 1, 2, \dots, n_w, \\ \epsilon_{ij} \mid \epsilon_{ij} = 1 - \delta_{ij}, ; \forall (i, j) : w_i, w_j \in W_T, i \neq j. \end{cases}, \quad (21)$$

where n_w is the graph's vertex count, and ϵ_{ij} denotes an edge connecting vertices w_i and w_j . The set E_T is defined using the Kronecker delta δ_{ij} to indicate that ϵ_{ij} is an edge if and only if $i \neq j$.

Furthermore, let V(T) be the volume occupied by the cellular structure driven by the skeletal graph T. Ideally, to achieve volume conformality, the volume difference between V(T) and V should be minimized. Thus, the volume conformity can be expressed as:

$$\Delta V = |V - V(T)| \to \min.$$
⁽²²⁾

The use of a skeletal graph promotes a more stable structure with enhanced mechanical properties, ensuring more even load distribution, thus reducing stress concentrations and potential failure points. To evaluate the uniformity of the cellular structure within the volume V, a uniformity metric \mathcal{U}_m is introduced:

$$\mathcal{U}_m(T,V) = \frac{1}{|V|} \int_V |\nabla T - \nabla V|, dV, \qquad (23)$$

where ∇T and ∇V are the gradients of the skeletal graph and the volume, respectively, and |V| is the total volume. This metric helps assess how uniformly the cellular structure fills the designated volume.

The uniformity of the cellular structure within the volume V can be mathematically represented as follows:

$$\mathcal{U}(V) = \sum_{\epsilon_{ij} \in E_T} \frac{1}{|E_T|} \left| \frac{\partial W}{\partial \epsilon_{ij}} \right|,\tag{24}$$

where $\frac{\partial W}{\partial \epsilon_{ij}}$ denotes the volume change due to an edge ϵ_{ij} change.

This approach may result in abrupt beam cuts in cellular structures. Let α be the percentage of these abrupt cuts, which ideally should be minimized for a seamless cellular structure:

$$\alpha = \frac{\text{Number of abrupt beam cuts}}{\text{Total number of beams in the skeletal graph}} \times 100\%.$$
 (25)

To counter this, the net-skin method is introduced to cellular structures, integrating the skeletal graph representation. A net-skin is applied to a cellular structure to alleviate adverse impacts of trimming [79].

The net-skin method is beneficial for creating conformal cellular structures with complex geometries and optimizing the mechanical properties of a structure. It is especially useful for crafting structures with non-uniform strut orientations, connectivity, and sizes, which can significantly influence the mechanical properties of a structure [79].

2.4. An exploration study of the geometric modeling of heterogeneous cellular structures with multiple surface-based topologies

In the realm of geometric modeling, achieving topology transition in cellular structures holds critical importance. Traditional techniques have been primarily dominated by subdivision surfaces, a potent instrument from computer graphics, employed to derive smooth surfaces from coarse meshes. This approach utilizes subdivision to refine meshes, and subsequently employs smoothing algorithms to render a smooth topology [80]. This explorative study, however, ventures beyond this well-trodden path and innovatively introduces an approach that interpolates between multiple topologies within a heterogeneous cellular structure. Moreover, the proposed method stands out by leveraging skeletal graphs, which, as established earlier, are crucial for representing the intrinsic connectivity of cellular structures. This connectivity representation acts as the guidance for the interpolation process across different topologies, marking a novelty in the proposed approach.

Elaborating further, consider two distinct topologies, T_1 and T_2 , as illustrated in Fig. 5(a), separated by a gap denoted by δ . Introducing x as an axis originating from T_1 and culminating in T_2 , perpendicular to their respective surfaces, the goal is to define their outer faces, T_1^+ and T_2^- , in relation to this axis. By extrapolating the contour curves of these topologies, represented as ∂T_1^+ and ∂T_2^- , it is proposed to interpolate the transition region, δ , based on these contours. Importantly, the skeletal graphs of each topology are pivotal in guiding this interpolation.

The interpolation between the two contours can be expressed by a parameter λ , which varies from 0 to 1. For any point A on ∂T_2^+ and its corresponding point B on ∂T_2^- the interpolated point C can be defined as:

$$C(t) = (1 - \lambda)A + \lambda B, \quad 0 \le t \le 1.$$
(26)

This equation linearly interpolates between the points A and B, producing a transitional morphology between the topologies.

Note that ∂T_1^+ and ∂T_2^- are not necessarily closed curves. For instance, a cross-section of a face of the Schwarz P unit cell topology is a closed circular shape. However, this proposed approach aims to cover cases where the unit cells are not complete. For example, a cross-section of half of the Schwarz P surface unit cell is represented by four differently oriented open curves. Thus, $T_{1\#2}$ may comprise disconnected surfaces. The interpolated connection between two solid bodies defined with surfaces may not be trivial and could lead to visual artefacts [82]. It is proposed to mitigate this effect by splitting topology faces T_1^+ and T_2^- into quarters, assuming the origin is at the centroid of the faces. Let I_+ , II_+ , III_+ , and IV_+ represent the quarters on the T_1^+ face, or positive quarters, and I_- , II_- , III_- , and IV_- represent the quarters



Figure 5: Geometric modeling of cellular structures with multiple surface-based topologies. (a) A schematic depiction of the transition between topologies T_1 and T_2 with (b) the transition region $T_{1\#2}$ in the gap δ between topologies T_1 and T_2 , (c) a wireframe transition between skeletal graphs of a gyroid and a Schwarz P topologies, (d) a surface-based cellular structure transition between the gyroid and Schwarz P topologies with the thickness of the structure varying vertically, and (e) a screenshot from the Preform software [81] validating the printability of the TPMS transition structure created using the proposed approach.

on the T_2^- face, or the negative quarters. The proposed approach is to connect curve sections in positive quarters to their corresponding sections in negative quarters. In this method, $T_{1\#2}$ is viewed as a skeletal graph derived from the two neighboring graphs.

To address the complexity in connecting open curves of different topologies, a curvature-matching function $M(\partial T_1^+, \partial T_2^-)$ is proposed:

$$M(\partial T_1^+, \partial T_2^-) = \sum_{i=1}^n \min_j \left| \kappa_i(\partial T_1^+) - \kappa_j(\partial T_2^-) \right|, \qquad (27)$$

where κ_i and κ_j are the curvatures of points on ∂T_1^+ and ∂T_2^- , respectively.

This function aims to minimize the curvature difference between corresponding points, ensuring a smoother transition.

For a more gradual and controlled transition between the topologies, a blending function $H(\lambda)$ can be introduced:

$$H(\mathbf{X}) = 3\mathbf{X}^2 - 2\mathbf{X}^3,\tag{28}$$

which is a smooth step function, commonly used in computer graphics for blending. It ensures a smooth transition from T_1 to T_2 by gradually changing the influence of each topology [83]. This function assists in governing the weight or influence of each topology within the transition region. It can be formulated using several mathematical representations, like quadratic or cubic interpolating functions, tailoring to the specific nature of the desired transition. The conditions H(0) = 0 and H(1) = 1 must be satisfied by $H(\mathbf{X})$ to ascertain a flawless and uninterrupted transition.

The proposed method presumes regular tessellation of T_1 and T_2 and assumes $\partial T_1^+ \parallel \partial T_2^-$. The incorporation of irregular tessellations remains a potent area for further exploration, and this study plants the seed for such prospective research endeavors.

3. Implementation

This section shifts the focus from theoretical exploration to the practical implementation of the advanced cellular structures delineated in Section 2.1. Utilizing the foundational concepts of F-rep and skeletal graphs, this section details the application of these methods within the LatticeQuery framework [84], a versatile and open-source software that integrates CadQuery [85], CQ-editor [86] and OpenCASCADE [87] for robust geometric modeling. LatticeQuery, characterized by its open-source nature and adaptability, serves as a testbed for implementing and validating the modeling approaches proposed in this study.

LatticeQuery stands out for its ability to model complex cellular structures, granting users a high degree of control over the geometric aspects via the F-rep approach. Unlike many commercial solutions, the open-source nature of LatticeQuery reduces costs [88] and welcomes improvements from the broader community. Further, the software is adept at creating both stochastic and conformal cellular structures, meeting the varied needs of industry applications.

This section is organized into subsections, each dedicated to a distinct aspect of cellular structure implementation. Subsection 3.1 delves into the practicalities of creating stochastic cellular structures, demonstrating the application of the proposed methodology through the generation of Voronoibased designs. This is followed by Subsection 3.2, which elaborates on the development of conformal cellular structures, focusing on both surface (Subsection 3.2.1) and volume conformality (Subsection 3.2.2). These subsections collectively demonstrate the capacity of LatticeQuery to model structures that conform precisely to pre-defined surfaces and volumes, showcasing its utility in diverse industrial contexts. Lastly, Subsection 3.3 highlights the technique for transitioning between different surface-based cellular structures, underscoring the adaptability and efficiency of the proposed approach in handling complex multi-topology transitions. Through these implementations, this work aims to bridge the gap between theoretical models and their practical applications, providing insights into the real-world feasibility and utility of the proposed geometric modeling techniques.

3.1. Stochastic cellular structures

In this work, SciPy [89], a Python library well-suited for numerical operations with graphs, is leveraged to implement the skeletal graphs of stochastic cellular structures. This enables the modeling of Voronoi cellular structures [90, 91]. SciPy can generate a defined number of Voronoi seeds and compute their corresponding Voronoi cells in 3D. For modeling stochastic structures, users need to supply parameters like the number of Voronoi seeds, the desired lattice thickness, and the boundary of the object to be filled. Given that both LatticeQuery and SciPy are Python libraries, they can be co-implemented to model stochastic cellular structures.

The process begins with the generation of Voronoi seeds within a predefined three-dimensional space. This step is crucial as it sets the foundational layout of the cellular structure. In the implementation, a specified number of seeds are distributed randomly, ensuring a stochastic arrangement. The SciPy library, with its spatial algorithms, is then employed to compute the Voronoi diagram based on these seeds.

Once the Voronoi diagram is established, the next phase involves the detailed computation of the edges between neighboring Voronoi cells. These edges are critical as they form the skeletal framework of the cellular structure. SciPy facilitates the extraction of these edge coordinates, which are pivotal in defining the geometric boundaries of each cell. SciPy computes the edges between neighboring Voronoi cells and provides their coordinates. This data can be used to generate equations of line segments, which can be fed into LatticeQuery. These equations form the topology-defining function T. Following this, the parameter-defining function P can be applied to provide additional properties such as lattice thickness. Figures 4(c) and 4(d) demonstrate a Voronoi cellular structure that fills the volume of a human femur bone, which was imported in the STL file format. Figure 4(e) shows stochastic Voronoi structures modeled using the proposed approach that conform to random polyhedrons.

The integration of LatticeQuery and SciPy enables a seamless transition from the computational generation of cellular structures to their practical modeling. This synergy is particularly beneficial for creating stochastic structures that conform to specific geometric boundaries, as demonstrated in the case of the Voronoi cellular structure filling the volume of a human femur bone.

As mentioned in Section 2.2, the graph representation of a cellular structure is beneficial for estimating its mechanical and physical properties. Future improvements could focus on optimizing seed generation for more controlled cellular structures, implementing advanced algorithms for boundary condition management, and enhancing the interface of LatticeQuery for a more intuitive modeling experience. Additionally, future research could explore incorporating the graph representation as metadata alongside the geometry itself within a CAD file format.

3.2. Conformal cellular structures

This section discusses the intricacies of implementing conformal cellular structures, with a focus on surface and volume conformality, detailed in Section 3.2.1 and Section 3.2.2, respectively. These subsections give a comprehensive view of the practical use of the proposed function representation approach to design conformal cellular structures with specified surface and volume characteristics. By outlining the implementation process and its implications, this section displays the versatility and efficacy of the proposed approach when dealing with the complexities of conformal cellular structures, thus providing the foundation for improved design and performance in various industrial applications.

3.2.1. Surface conformality

The method highlighted in Section 2.3 is implemented in LatticeQuery through the integration of NumPy [92] numerical operations. The implementation process starts by defining a surface equation that the cellular structure will conform to. A simple cubic topology is used as an example, conforming to a mathematically defined surface. In this case, the surface is described by a sinusoidal equation, providing a non-linear, wave-like geometry:

$$\Phi(\mathbf{X}): y = \frac{5\sin(x)}{x} \text{ for } x \in [-25, 25], z \in [0, 15].$$
(29)

The next step involves the definition of the function P, which regulates properties such as beam thickness across the topology. This is where the NumPy library allows for the manipulation of these properties based on mathematical functions. In the example, the function P is defined to regulate the beam thickness t as:

$$P(\mathbf{X}): t(x) = 0.125 + |0.025x|.$$
(30)

Let $N_x = 18$, $N_y = 5$, and $N_z = 2$ represent the numbers of unit cells along the x-, y-, and z-axes, respectively. Assume one layer of unit cells along y to be of the normal distance h/2 = 2 mm. The method requires the normal vector field defined for $\Phi(\mathbf{X})$. This field can be obtained by rotating the tangent vector by $\pi/2$ and normalizing it. The tangent vector can be calculated from the derivative of Φ , which corresponds to the slope of the tangent line at any point on the curve:

$$k = \frac{\partial \Phi(\mathbf{X})}{\partial x} = \frac{x \cos(x) - \sin(x)}{x^2}.$$
(31)

The farthest equidistant surfaces Φ_+ and Φ_- from the middle plane Φ are numerically derived from the slope of the normal line, which is the negative reciprocal of the slope of the tangent line, or

$$-\frac{1}{k} = -\frac{x^2}{\sin(x) - x\cos(x)}.$$
(32)

The normal line equation with the normal distance h/2 = 2 mm can be derived. For all $(x_k, y_k, z_k) \in \Phi(\mathbf{X})$, the corresponding points of the equidistant

surfaces Φ_+ and Φ_- can be determined from the Euclidean distance and the normal line equation as a solution of

$$\begin{cases} (x - x_k)^2 + (y - y_k)^2 = \left(\frac{h}{2}\right)^2, \\ y - y_k = \frac{1}{k}(x - x_k), \end{cases}$$
(33)

which results in this case to

$$x = \frac{2B \pm \sqrt{(2B)^2 - 4AC}}{2A},\tag{34}$$

where $A = 1 + \frac{1}{k^2}$, $B = x_k + \frac{x_k}{k^2}$, and $C = x_k^2 + \left(\frac{x_k}{k}\right)^2 - \left(\frac{h}{2}\right)^2$. The two solutions correspond to Φ_- and Φ_+ , as they are both equidistant to Φ . The resulting structure of this example is showcased in Fig. 3(c).

3.2.2. Volume conformality

As indicated in Section 3.1, in the volume conformality process, the primary objective is to fill a predefined volume with a cellular structure that precisely conforms to its boundaries. This volume is typically represented by an imported STL file, which serves as a template for the desired shape. The initial step involves using NumPy to create a dense grid of points within the volume. This grid represents potential vertices for the cellular structure and is the foundation upon which the conformal structure will be built.

The trimming process is crucial in ensuring that the cellular structure conforms to the exact shape of the volume. This is achieved by identifying the vertices within the grid that intersect the boundaries of the STL file. By pinpointing these intersections, the algorithm can determine which edges need to be trimmed to fit the volume precisely. The identification of these vertices and edges involves spatial computations, which are facilitated by the mathematical capabilities of NumPy.

Once the necessary vertices and edges are identified, the next step is to implement the sweep method from the Open CASCADE [87] geometric modeling kernel. This method is essential for creating smooth and continuous connections between the vertices, particularly at the trimmed edges. By employing the sweep function, the algorithm can generate surfaces that seamlessly bridge the gaps between the trimmed edges and the boundaries of the STL file.

This implementation approach addresses the challenge of creating a cellular structure that not only fills the volume but also adheres to its complex geometrical features. The refinement process involves iteratively adjusting the positions of the vertices and the paths of the edges to ensure a snug fit within the volume. This refinement is computationally intensive and requires careful consideration of the geometrical and topological properties of both the cellular structure and the STL file.

By refining the volume conformality implementation, a more accurate representation of the cellular structure within the desired volume can be achieved. This refinement sets the stage for enhanced performance and dependability in a variety of applications. Figure 4(e) depicts the refined conformal stochastic structure that occupies the volume within a human femur bone, imported in the STL file format.

3.3. Topology transition between surface-based cellular structures

The topology transition methodology outlined in Section 2.4 seeks to fill a gap δ between surface-based structures. It is proposed to fill the space between unit cells of topologies T_1 and T_2 with a quasi topology $T_{1\#2}$.

The implementation begins by defining the geometry of the initial and final topologies, T_1 and T_2 . This involves creating a detailed wireframe model for each topology, where the wireframe is a skeletal graph representation of the cellular structure. The wireframe models are generated using algorithms that accurately represent the intricate geometrical features of each topology.

The next step is to identify the boundary curves, ∂T_1^+ and ∂T_2^- , of these topologies. These curves are critical for the interpolation process, as they define the transition zone, δ , between T_1 and T_2 . To achieve this, advanced algorithms compute the intersecting lines or curves between the adjacent topologies, ensuring the transitional area accurately reflects the characteristics of both topologies.

Once the boundary curves are established, the algorithm then interpolates the space between them, creating the quasi-topology $T_{1\#2}$. This interpolation is not a straightforward linear process but involves geometric calculations that account for the curvature and orientation of the boundary curves. The result is a smooth and continuous transition between the two different topologies.

The implementation further refines this process by applying varying geometric parameters, such as thickness and density, across the transition zone. These parameters are modulated using function P, which allows for a high degree of control over the physical characteristics of the transitional structure. This ensures that the final structure not only visually transitions between the topologies but also maintains functional integrity across the transition.

The practical application of this methodology is demonstrated in Figure 5(d), where a cellular structure transitions between a gyroid and a Schwarz P topology. The illustration shows how the structure's thickness varies vertically, showcasing the effectiveness of the approach in creating complex, multi-topology structures.

A benchmarking test was conducted to evaluate the performance of the geometric modeling software on this cellular structure. The test was performed on a system equipped with an AMD Ryzen 7 3700X central processing unit (CPU), an NVIDIA GeForce RTX 2070 Super GPU, and 32GB of available random-access memory (RAM), running Arch Linux with a kernel version of 6.6.8-arch1-1. During the execution, the software demonstrated significant computational efficiency, with an average CPU usage of 83.9% and RAM usage of 30.5%, indicating robust utilization of the available processing capabilities. The GPU performance was also noteworthy, with 2748.0MB of its total 8192.0MB memory being actively used, leaving 5217.0MB free, which suggests effective management of graphical processing resources. The execution time for the modeling process was recorded at 528.48 seconds, showcasing the capability of the software to handle intricate geometric computations within a reasonable timeframe. This benchmarking exercise highlights the potential of the software in efficiently managing system resources while performing complex geometric modeling tasks, making it a viable tool for advanced cellular structure design in computational environments with similar specifications. Nevertheless, the solid model generation process can be potentially optimized by implementing GPU acceleration techniques [93].

The traditional method models TPMS structures by constructing one octant of a unit cell and tessellating for optimization purposes, a technique in line with the object-oriented programming (OOP) method [94]. This implies that the conventional technique of modeling one octant and tessellating it would not be applicable for transitional unit cells. Moreover, as highlighted in Section 2.4, the boundary curves ∂T_1^+ and ∂T_2^- are not necessarily closed. As a result, a simple loft CAD feature between ∂T_1^+ and ∂T_2^- does not sufficiently address general non-trivial cases [95]. Figure 5(d) displays the transition between the gyroid and Schwarz P topologies while concurrently varying the structure thickness in a different direction.

Important properties of geometric modeling are the mesh quality of the output solid model and the assessment of its manufacturability. To highlight the direct applicability and practical relevance of the proposed methodology, a screenshot of this TPMS transition structure, as visualized in the Preform software [81], is showcased in Fig. 5(e). This demonstrates the compatibility of the generated structures with standard STL formats and sufficient mesh quality, making them readily usable for AM. Note that additional support structures can be required to compensate for overhanging of regions of some structures. Importantly, the printability check has been successfully passed, underpinning the robustness of the proposed approach. Additionally, the manufacturability assessment approach developed by Zhang [96] has been applied to the resulting solid model and confirms its manufacturability with quantitative metrics.

4. Conclusion

This paper introduces a novel approach to modeling cellular structures using function representation (F-rep) combined with the LatticeQuery opensource tool. The proposed method enhances the geometric modeling capabilities for a wide range of cellular structures, encompassing stochastic, conformal, and transitional topologies between surface-based structures. This versatility allows for the creation of cellular structures that are not only complex in design but also capable of smoothly transitioning between different forms.

The proposed approach marks an advancement in the field of geometric modeling, offering designers the flexibility to create more efficient and customized structures. This adaptability is particularly beneficial in applications where performance and specificity of design are paramount. By enabling the creation of cellular structures that seamlessly fit into complex designs and smoothly transition between them, the proposed method opens new approaches to generate innovative and high-performance designs.

Looking ahead, the future research directions include exploring a wider array of cellular structure types and their potential applications, thereby enhancing the versatility and utility of LatticeQuery and the proposed modeling method. There is also a significant opportunity in developing advanced strategies for estimating the mechanical and physical properties of cellular structures directly from their graph representations. This will facilitate rapid and accurate performance assessments during the design phase, significantly improving the design-to-production workflow. Additionally, investigating the integration of the proposed method with existing CAD systems will enable designers to leverage familiar tools and workflows while benefiting from the advanced capabilities of the proposed approach. Furthermore, exploring the application of machine learning and optimization algorithms to automate the creation of cellular structures will allow for designs that are optimally tailored to specific requirements and constraints, pushing the boundaries of what is currently achievable in geometric modeling.

By building upon the foundational work presented in this paper and leveraging the capabilities of the open-source software developed, the research community is positioned to forge new paths in the design of advanced cellular structures. These developments hold the promise of significantly improved performance and a wide range of applications, driving innovation in geometric modeling and beyond.

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