Shape-Dependent Self-Assembly Metamaterial with Aperiodic Microstructures

Introduction: Recent advancements in technology have enabled new ways of constructing metamaterials that possess desirable mechanical properties. Materials that have high elastic stiffness and low density are considered some of the strongest, stiffest, lightest materials available today [1]. By controlling their microstructures, we can tune mechanical properties of metamaterials that endure extreme conditions.

A trait of a metamaterial microstructure that is much ignored to date is randomness (aperiodicity), owing to the limitation of current design approaches based on unit cells. Aperiodic structures are likely to result from natural self-assembly and self-organization processes and may be more robust against uncertainty. Examples of robust microstructures can be seen in natural formations such as wood and nacre, or in parts of the human body such as bone [2]. Materials that are robust against uncertainty perform well under various forces and stresses they may encounter.

Currently, state-of-the-art approaches for designing metamaterial microstructures for desirable properties can be categorized either as parameterized design or topology optimization methods. Both approaches build their foundation on the assumption that material microstructure consists of periodically repeated motifs (or unit cells). Parametrized design is a simpler design method to design structures like lattices; it allows for a few design parameters to map directly to specific properties, but it needs an ad-hoc design to start with. Since the design space is quite narrow, there is a narrow range of achievable material property ranges. Meanwhile, topology optimization is a design method that allows for freeform design of a structure with almost any geometry; it is mathematically well defined, but computationally expensive, leading to unpredictable geometries that are hard to manufacture [3]. Both approaches are difficult to use as tools to efficiently and effectively explore the vast design space of material microstructures.

By combining optimal features of each method, this research aims to expand the microstructure design space to maintain local parametric behavior while enabling global freeform design. Through numerical approaches, one can program aperiodic material microstructures towards desirable properties using a "growth"-like process that is encoded by "DNA"-like pairwise combination rules. With this "growth" process, a method for physical self-assembly is desired as it allows for rapid production of programmable metamaterials. The mechanical self-assembly process has been explored in several applications across different scales [4, 5], but none have been able to achieve mechanical self-assembly of an aperiodic microstructure. This design approach allows us to efficiently generate new random yet ordered microstructures. It enables effective exploration of the material design space and pushes the boundaries of applying new stronger materials to applications such as shock absorption and acoustics.

Research Plan: I aim to develop self-assembly methods to investigate how the shape and design of cellular automata base cells affect mechanical properties of programmable metamaterials. I will then develop specific tunable metamaterials for applications that desire the particular properties. Numerical, experimental (Fig. 1), and application phases can be achieved with FEA software, 3D printing, and mechanical testing equipment commonly used in any mechanical engineering lab. My previous research experience doing this with square-shaped tiles demonstrates my technical capability.

***Specific Aim I. Develop Baseline Samples*:** I will first develop a wave function collapse algorithm [6] for various polygons, such as pentagons and hexagons. The versatile algorithms will be developed in Python for both 2D and 3D self-assembly with flexibility for varying polygons. To do this, I will use a so-called wave function collapse algorithm, which performs a "growth" process similar to cellular automata. We define fundamental building blocks and connectivity rules over a cellular space. Once the first cell is set, connectivity rules are enforced to determine surrounding cell states; this process then repeats in

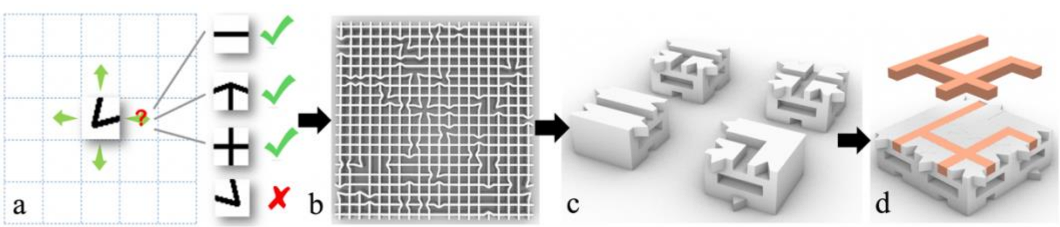

Figure 1. Proposed workflow: **a)** develop cellular-automata algorithm, **b)** generate baseline sample, **c)** create self-assembly tile method, **d)** fabricate experimental metamaterial.

propagating cycles. This will generate 2D and 3D samples for multiple shapes to be transformed into 3D objects in Rhino with Grasshopper C# that will be tested using FEA software. This forms a baseline mapping of the programmable microstructure design space as a success assessment.

Specific Aim II. Perform Physical Experiments: From my numerical analysis of these structures, I will 3D print specific samples generated by the algorithms and physically perform the same mechanical tests as in the numerical phase using mechanical testing equipment, such as an Instron machine. The results of these tests can be compared to the numerical results to evaluate their degree of error.

Physical 2D and 3D self-assembly methods for multiple shapes will be developed to gain further insight into this self-assembly method. Inspired by the mechanics of DNA self-assembly processes [7], I will design tiles for each shape with their respective channel types dictated by the polygon's interior angle. This tile design and experimental setup must ensure some randomness and adhere to the algorithm-determined connectivity rules. The self-assembled 3D printed tiles will be used as a carrier casting mold in which to pour a plastic material to generate the metamaterials to be tested. Using the same mechanical testing methods as the previous samples, I will then compile and analyze data for information about the design space and microstructure properties with a focus on how base cell shape and corresponding interior angles affect mechanical properties of the metamaterial microstructures. At this point, a new physical method for developing aperiodic programmable metamaterials will have been created. The design space can be studied by constructing a material database. If the physical self-assembly method is not experimentally reliable, the initial algorithm-based numerical study and mechanical tests still provide a wealth of data to be used in the applications phase.

Specific Aim III. Develop Metamaterials for Applications: Based on my findings from the studies performed in the previous phases, I will then study special properties of certain metamaterials that this self-assembly method yielded, such as shock absorbency and acoustic capacity. My experimental results will yield a desired mechanical property by tuning the specific base cell shape and quantity of channel type. With these settings, the physical self-assembly method can be used to create an array of samples used for additional testing for specific properties, such as impact testing in the shock absorbency case. These studies will demonstrate how the metamaterials yielded from the developed self-assembly method can be applied as lighter, stronger, and more flexible alternatives to materials currently used in aerospace and medicine.

Intellectual Merit: This project will develop a mechanical self-assembly method of aperiodic programmable metamaterials, contributing new 2D and 3D self-assembly methods to metamaterials and mechanics research; this will improve the fundamental understanding of material microstructures and their properties. This project will also enhance understanding of the mechanics of self-assembly such as attractive forces and interlocking as seen in DNA self-assembly [7]. Working on this project at a research institution with a strong mechanical engineering program will provide the proper resources to research and publicize my findings related to metamaterials, bio-inspired processes, and their applications to medical and aerospace fields.

Broader Impacts: This project will contribute new 2D and 3D self-assembly methods to metamaterials and mechanics research while developing new aperiodic programmable metamaterials with large degrees of tunability. Scale-independent metamaterials will be created that can be applied to aerospace materials, soft materials, and medical devices for its capabilities of enhanced shock absorbency, acoustic properties, elasticity, and strength. Additionally, through its biologically linked process of self-assembly, the microstructures developed have the potential to be applied to sustainable, environmentally friendly structures and devices. This project also has a parallel educational impact to introduce high school and undergraduate students to numerical and experimental methods in mechanical engineering and STEM. I plan to mentor students in researching metamaterials.

[1] J. B. Berger et al., "Mechanical metamaterials," pp. 533–537. [2] H. Wagner et al., "Bone microstructure," pp. 1311–1320. [3] O. Sigmund et. al, "Topology optimization," pp. 1031–1055. [4] E. Klavins, "Programmable Self-Assembly," pp. 43–56. [5] G. M. Whitesides, "Self-Assembly," pp. 2418–2421. [6] Heaton, R. (2018). Wavefunction Collapse Algorithm. [7] S.-S. Jester et al., "DNA nanostructures," pp. 1700–1709.