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Computational challenges in additive manufacturing for metamaterials design

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Additive manufacturing plays an essential role in producing metamaterials by precisely controlling geometries and multiscale structures to achieve the desired properties. In this Comment, we highlight the challenges and opportunities from additive manufacturing for computational metamaterials design.

Metamaterials are engineered structures with properties not typically found in natural materials, achieved through their unique micro- or nano-scale architecture. Additive manufacturing (AM), or 3D printing, plays a crucial role in creating these complex structures[1]. It allows for precise control over the material's geometry at the scale necessary for metamaterial properties to emerge. The additive nature of 3D printing can construct intricate patterns and shapes required to achieve the desired metamaterial behavior by enabling rapid prototyping, customization, and the ability to explore a vast design space with relative ease and efficiency. Further, emerging '4D printing' techniques, which incorporate time as a fourth dimension, can lead to features or properties (for example, shape, stiffness, and so on) that are programmed to evolve and adapt to environments after production[2]. However, designing and predicting the behavior of additively manufactured metamaterials is complex because their properties are dependent upon physical phenomena that can be highly sensitive to minute structural details at multiple length scales and processing parameters. In this Comment, we will discuss the computational challenges and opportunities associated with additive manufacturing for metamaterials (see the schematic in Fig. 1, top).

The first challenge is the vast design space offered by AM, magnified by the hierarchical nature of metamaterials, which makes brute-force design exploration impractical. Recent strides in research have suggested using graph-based representations to better capture the irregularities within material architectures, thereby providing a more accurate depiction of potential design variations[3]. Additionally, parametric or procedural designs leverage algorithms to generate structures based on a limited set of initial parameters, simplifying the

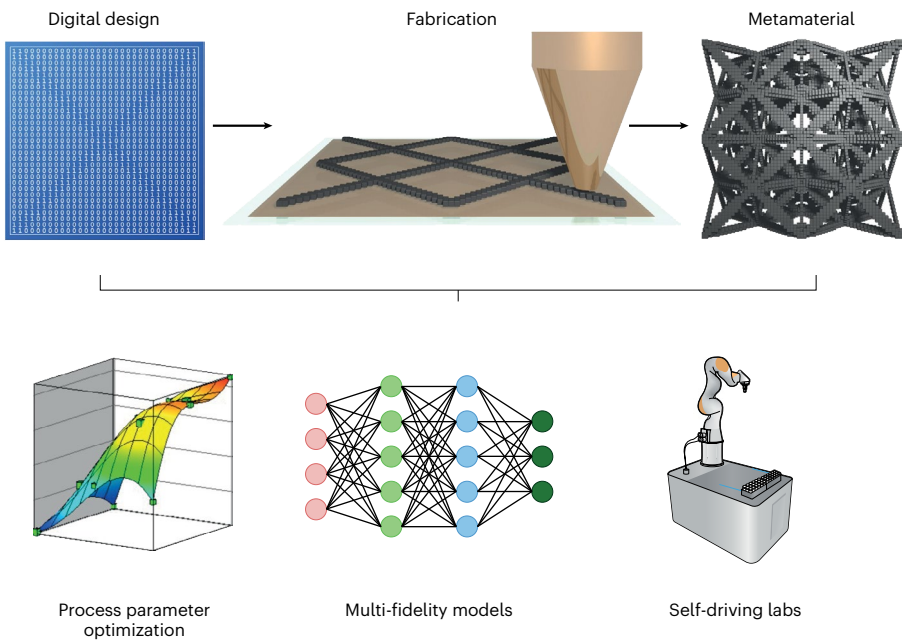

Fig. 1 | The additive manufacturing process for metamaterials fabrication and highlights of the emerging techniques that can assist the production of metamaterials. Top: the conventional additive manufacturing (AM) process for metamaterials includes mapping out the digital design space and the printing process for fabrication. Bottom: methods that can help in the design of AM for metamaterials design and validation. Process parameter optimization methods for optimizing the multi-dimensional parameter space in AM (left). Multi-fidelity machine learning models for incorporating architectural design and process parameters into computational models (middle). Self-driving labs for automated exploration of complex metamaterial design spaces (right). The green dots represent selected points on the 3D plot and the colours in the multi-fidelity model represent different layers in the neural network.

design process. To effectively navigate this extensive design space, optimization techniques such as topology optimization and genetic algorithms are employed[4]. Machine learning also plays a crucial role by enabling generative design strategies that can predict complex architectures from a relatively modest input of variables, thus expediting the design process. Another innovative approach involves utilizing self-assembly processes to naturally dictate the formation of finer-scale features[5]. Addressing the AM constraints, such as support material requirements and printer resolution, is integral to the computational design process. Previous approaches have managed these constraints by incorporating simulation tools that predict the need for support structures and adjust the design to optimize resolution and material use[6]. These simulations and related computational tools are essential for optimizing the use of support structures, which are often necessary to prevent the collapse of overhanging features and to maintain the integrity of the structure during the printing process. By accurately predicting where supports are needed, simulation tools and algorithms can help reduce the amount of excess material used, thereby minimizing waste and decreasing the post-processing time required to remove these supports. By blending advanced computational methods with practical manufacturing considerations, the field can push the boundaries of what is possible with metamaterials in AM.

Another challenge for computation is the effect of processing conditions and parameters on the additively manufactured metamaterial part. The mechanical properties of parts produced through additive manufacturing are influenced by process parameters and conditions such as energy input, layer height, printing speed, and ambient conditions (with specifics that depend on the AM approach)[7]. These printing parameters can affect the microstructure of materials, which in turn impact the strength, ductility, and fatigue life of the printed parts. Recently, there have been in situ monitoring and correction techniques developed to detect these effects and correct for them[8]. Computational models must incorporate these variables to provide accurate predictions of the final product's properties. By simulating the additive manufacturing process, taking into account the thermal history, stress development, and cooling rates, the models can be used to optimize parameters for desired mechanical outcomes (Fig. 1, bottom left). This predictive capability is essential for developing design principles that can reliably produce parts with specified properties and performance. Hence, the integration of process parameters into computational models or digital twins[9] is critical for advancing AM toward producing parts that meet precise engineering specifications and for the systematic exploration of new material systems and geometries. Digital twins, virtual replicas of physical systems updated with real-time data, can be conducive for simulating, predicting, and optimizing the AM process to achieve precise engineering specifications and explore new materials and geometries.

Ultimately, the integration of architectural design and process parameters into computational models would be key to obtaining metamaterials with desired properties and functionalities. When considering the data needed to train such models, there is a tradeoff between cost and fidelity, namely that high-fidelity simulations are often necessary to capture complex phenomena, but cheaper low-fidelity simulations are more appropriate for exploring the vast parameter space. Furthermore, experiments are often necessary to take into account intricate processing-property relationships and processing-dependent defects. Utilizing multi-fidelity machine learning models[10] (Fig. 1, bottom middle) presents a promising approach to integrate architectural design and process parameters effectively. These models can simultaneously process high-fidelity simulations and experimental data alongside lower-fidelity, computationally cheaper data, enabling more accurate and efficient predictions. This approach substantially enhances the ability to optimize metamaterial properties and functionalities, addressing the challenge of computational complexity while reducing the time and resource expenditure typically required for such tasks.

The final challenge is that computational models of additively manufactured metamaterials must be evaluated and refined as part of the design and validation process. This is a challenge both because many metamaterial properties of interest are expensive or inaccurate to simulate and additive manufacturing introduces variations in microstructure that are not reliably predictable. From a throughput perspective, estimating properties using simulation or other computational modeling approaches such as machine learning would be preferred as this can be faster and less expensive than experiment. However, there are major challenges in accurately simulating metamaterial properties. First, there are many properties for which accurate and fast computational predictors have yet to be developed[11]. For instance, it is very challenging to predict the high-strain mechanics of components due to material nonlinearities, structural nonlinearities, and dynamic self-contacts. Similar considerations make it challenging to predict fatigue life of metamaterials using computational means. For properties that can be predicted using simulation such as elastic modulus or Poisson's ratio, accurately capturing the hierarchical geometry with the processing-specific microstructure is challenging. If the metamaterial contains structural motifs that spans over three orders of magnitude in size, the numerical precision and minimum voxel size needed to capture these features from AM processes can make any simulation computationally expensive to run, motivating the development of multi-scale approaches[12]. Furthermore, simulating 4D printed metamaterials poses computational challenges due to their dynamic nature where properties evolve over time in response to external stimuli. Due to these challenges, there have been efforts to capture large databases of experimental mechanical performance and use these to build or refine predictive models of metamaterial properties.

The complexity of validating simulations of the extreme mechanical performance of metamaterials against experimental data adds another layer of difficulty. Experiment remains the gold standard for testing metamaterial designs and validating simulation tools. This is especially true in extreme mechanics, where simulation tools are incomplete, and fields like nanophotonics where manufacturing-induced variations can strongly influence the optical properties of nanostructures. Thus, the speed and efficiency of experimental testing become a paramount concern. Recently, self-driving labs, or automated experiments (Fig. 1, bottom right) in which the experiments are selected by machine learning, have become an essential tool for rapidly exploring complex metamaterial design spaces[13]. The use of active learning strategies such as Bayesian optimization allows them to identify superlative designs with 10–1,000 times fewer experiments than grid-based searching[14]. At present, self-driving labs have been employed principally in the mechanics of additively manufactured structures and materials discovery, so there are many opportunities for developing systems to accelerate the study of many other facets of metamaterial design. For example, a single unified system that autonomously tunes material properties, produces hierarchical structures, and then functionally evaluates the resulting metamaterial has yet to be realized. The recent demonstration of a system that screens both material properties and architecture to study extreme mechanical properties provides inspiration for what type of superlative performance can be uncovered by simultaneously tuning material property and structure[15].

In closing, the frontier of metamaterials science represents a convergence of advanced additive manufacturing techniques, computational innovations, and experimental validation. As we harness the power of optimization, machine learning, and automated experimentation, the potential of metamaterials continues to expand, promising new application spaces.

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Competing interests

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