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Xiaohao Sun
The George W. Woodruff School of Mechanical Engineering,
Georgia Institute of Technology,
Atlanta, GA 30332
e-mail: xiaohao.sun@gatech.edu

Kun Zhou
Singapore Centre for 3D Printing,
School of Mechanical and Aerospace Engineering,
Nanyang Technological University,
50 Nanyang Avenue, Singapore 639798
e-mail: kzhou@ntu.edu.sg

Frédéric Demoly
ICB UMR 6303 CNRS,
Belfort-Montbeliard University of Technology (UTBM),
90010 Belfort, France;
Institut universitaire de France (IUF),
Paris, France
e-mail: frederic.demoly@utbm.fr

Ruike Renee Zhao
Department of Mechanical Engineering,
Stanford University,
Stanford, CA 94305
e-mail: rrzhao@stanford.edu

H. Jerry Qi[1]
The George W. Woodruff School of Mechanical Engineering,
Georgia Institute of Technology,
Atlanta, GA 30332
e-mail: qih@me.gatech.edu

Perspective: Machine Learning in Design for 3D/4D Printing

3D/4D printing offers significant flexibility in manufacturing complex structures with a diverse range of mechanical responses, while also posing critical needs in tackling challenging inverse design problems. The rapidly developing machine learning (ML) approach offers new opportunities and has attracted significant interest in the field. In this perspective paper, we highlight recent advancements in utilizing ML for designing printed structures with desired mechanical responses. First, we provide an overview of common forward and inverse problems, relevant types of structures, and design space and responses in 3D/4D printing. Second, we review recent works that have employed a variety of ML approaches for the inverse design of different mechanical responses, ranging from structural properties to active shape changes. Finally, we briefly discuss the main challenges, summarize existing and potential ML approaches, and extend the discussion to broader design problems in the field of 3D/4D printing. This paper is expected to provide foundational guides and insights into the application of ML for 3D/4D printing design.
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1 Introduction

Three-dimensional (3D) printing, or additive manufacturing, enables the creation of complex physical objects from digital models. Multimaterial printing allows for the fabrication of composite structures with materials of different properties and different active responses [1–3]. Owing to the development of multimaterial printing and active materials, the emerging 4D printing technology takes a step further by introducing time as a dimension, allowing printed objects to change their shape, properties, and/or functionality when exposed to specific environmental stimuli (e.g., light, heat, moisture, pH, solvent, and electric/magnetic field) [4–8].

There exist many 3D printing techniques. Depending on how the raw material is deposited, these techniques can be classified into the following categories: extrusion-based methods such as direct ink writing (DIW) and fused filament fabrication (FFF), jetting-based methods, vat-photopolymerization methods such as digital light processing (DLP), stereolithography (SLA), and two-photon polymerization (TPP), powder bed fusion-based methods such as selective laser sintering (SLS), etc. We refer the readers to recent reviews [8,9] for detailed descriptions of these techniques.

3D/4D Printing offers significant manufacturing flexibility, especially in creating complex shapes and structures that exhibit functions and responses beyond those of printed materials. Here, we refer to printed materials as those directly coming out of a printer without specially designed geometry or features; their properties are only determined by the printing techniques and printer operating parameters. In 3D/4D printing, design plays an important role in exploiting its advantage to enable intelligent printing and advancing various engineering applications [10–23]. This entails defining the functional description of transformable or deployable systems according to various usage scenarios, on which computational reasoning is needed to embody knowledge and decisions related to 4D printing. To achieve the appropriate geometry and structure of shape-changing

[1]Corresponding author.

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objects, decisions can be made on qualitative recommendation with the support of domain ontology (which is a component of symbolic artificial intelligence to formalize knowledge of an expertise domain with machine-interpretable description), as successfully demonstrated in the design of multimaterial 4D-printed objects [24,25].

However, addressing design for 3D/4D printing via symbolic reasoning alone is insufficient; it demands both the forward prediction of the properties, physical fields, load–displacement, and shape change of printed structures, and the inverse design of material distributions, topology, geometry, and stimulus fields (in terms of amplitude, location, and duration), as illustrated in Fig. 1. Printed objects can range from digital composites at the pixel (2D) or voxel (3D) level, to metamaterials or architected materials, and other active or intelligent material systems. Microstructures can also be encoded in pixels or voxels to create a hierarchical or multiscale material system [26,27]. The forward problem takes design inputs, such as material properties, material distributions, geometry, topology, hierarchies, and stimulus fields, and predicts mechanical-response outputs such as apparent structural properties (e.g., modulus, strength, toughness, and homogenized stiffness tensor for anisotropic hierarchical systems), physical fields (e.g., strain and stress fields), nonlinear load–displacement response and, particularly, the shape or function changes of active material systems (which can be seen as a deformation field). The inverse design problem seeks to find appropriate design inputs for tasks such as extremizing property values and obtaining designated properties or responses.

Motivated by the need to fully utilize the manufacturing flexibility, significant advancements have been made in developing design strategies. Topology optimization (TO) [28] represents a large class of methods that optimize the geometric features within a design domain to achieve certain objectives. While initiated for maximizing structural performance and minimizing weight, TO has found significant applications to a wide range of design problems in 3D/4D printing [29,30]. Examples include multiscale TO for enhanced structural performance [31–34] and programmed shape changes [35]; anisotropic composite TO for enhanced performance [36,37] and target actuated motions [38]; and TO for programming force-displacement response [39], shape changes of 4D-printed systems (such as active composites [40,41], inflatable structures [42], rod-based structures [43–45], and magnetoactive materials [46]), and continuous shape morphing paths or motions of soft composites [47,48]. In addition, TO has been used in the designs of supports and infills for improved part printability [29]. Despite its great success, TO generally requires complicated mathematical derivations and can be time-consuming due to computationally expensive physical simulations, especially when geometric and material nonlinearities are involved.

Machine learning (ML), particularly deep learning [49], offers an alternative approach that can handle complex mapping efficiently,

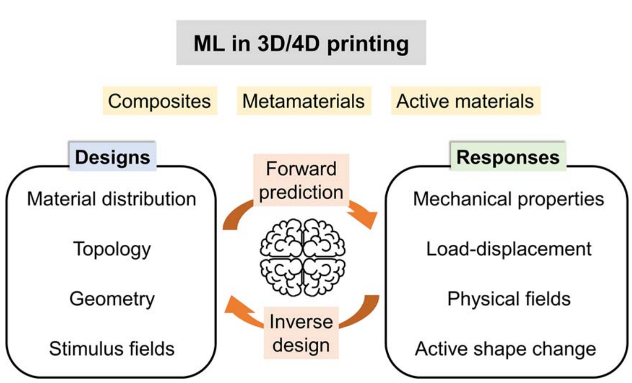

Fig. 1 Overview of forward and inverse problems in 3D/4D printing utilizing ML. The design space typically involves material distribution, topology, geometry, and stimulus fields. The output generally includes mechanical properties, load–displacement, physical fields, and shape change.

making it an attractive tool for the design of 3D/4D printing. ML can be broadly categorized into three types: supervised learning (SL), unsupervised learning (USL), and reinforcement learning (RL). SL learns the mapping in labeled data, which is often used for classification and regression tasks, such as property prediction. USL identifies inherent structures in unlabeled data, which may be used for clustering, dimensionality reduction, and discovering new structures. RL involves an agent that takes action in an environment to maximize a reward, which is often used for decision-making and optimization tasks. The landscape of ML techniques is vast and consistently evolving. Here, we list some popular methods used in design: support vector machine (SVM), decision tree (DT), neural network (NN), convolutional neural network (CNN), recurrent neural network (RNN), graph neural network (GNN), generative adversarial network (GAN), principal component analysis (PCA), variational autoencoder (VAE), Gaussian process (GP), Bayesian learning (BL), active learning (AL), and evolutionary algorithm (EA) among many others [50]. The readers are referred to textbooks [50] for working principles of these ML methods and to some recent reviews [51–53] for ML applications in the area of mechanics of materials.

In this perspective article, we review some recent works that apply ML methods to the design for 3D/4D printing. We primarily focus on the design of the mechanical properties or active responses of printed structures. While ML has many other applications in the entire field of 3D printing [54–58], such as processing parameter refinements [59,60], in-situ anomaly monitoring for quality control [61], and printing material design and discovery [62–65], these applications are not the focus here. The paper is organized as follows. Section 2 summarizes existing works on ML in 3D/4D printing designs, based on several categories of material systems and target properties/responses, and Sec. 3 provides discussions and perspectives.

2 3D/4D Printing Designs

2.1 Mechanical Properties of Composites. Composites that possess pixel- or voxel-level material distributions can be naturally encoded as number arrays, which are suitable for serving as input data for ML models. Extensive studies have been done on utilizing ML to predict or optimize various mechanical properties of composite (or heterogeneous) materials, such as effective modulus, strength, and toughness.

Cecen et al. [66] employed 3D CNN to predict the effective modulus of 3D heterogeneous materials. Li et al. [67] utilized CNN to predict the effective modulus of 2D heterogeneous materials. Regarding strength and toughness, Buehler and coworkers [26,68,69] have made significant efforts in exploring the ML capability in composite optimizations. They developed an ML classification model [68] to evaluate 2D composite designs in terms of their strength or toughness and distinguish them as either “good” or “bad.” The model, once trained with FE-generated data, can be used to assess the ranking of unseen designs, thus empowering the optimization to achieve high strength or toughness. The optimized designs based on this approach are shown in Fig. 2(*a*). An ML regression model [69] was later developed and combined with EA to optimize the composite strength and toughness under shear loading.

In composite designs based on pixels, the design space is often tremendous. To mitigate this issue, Buehler and coworkers [26] innovatively incorporated ML with the hierarchical design concept. This strategy uses specific microstructures containing numerous pixels as basic design units and then performs the prediction or design in a coarse-grain manner. As shown in Fig. 2(*b*), they proposed three elementary design units with different anisotropies. The ML model was then employed to predict the mechanical properties of the composite system, which, in turn, enabled fast optimizations. In addition to NN and CNN, the application of other ML methods such as active learning [74] and reinforcement learning [75,76] for the bioinspired composite designs has been explored. Furthermore, minimizing the overall compliance of irregular

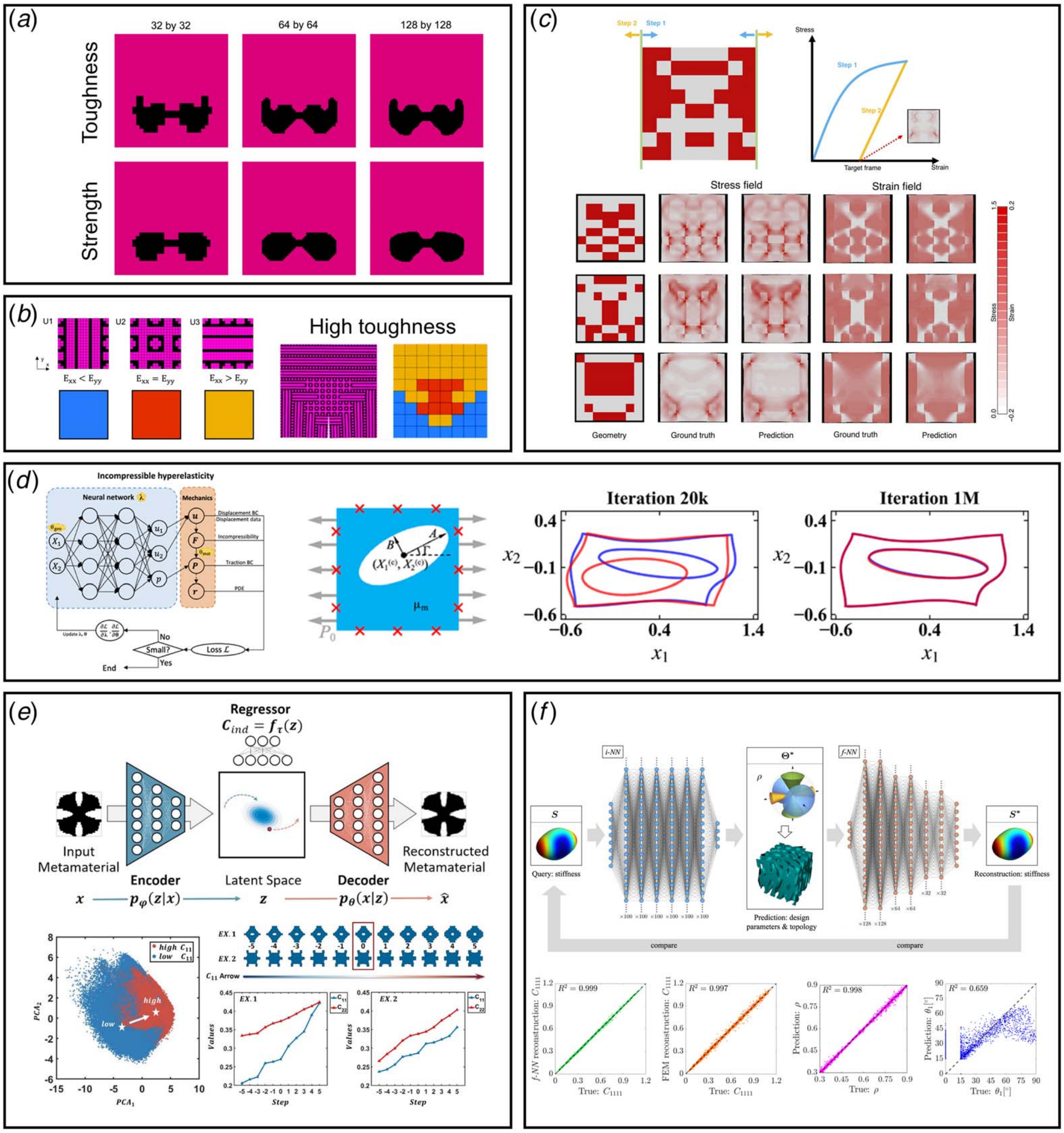

Fig. 2 Applications of ML in various material systems with different design parameters and mechanical responses. (*a*) Optimized material distributions of composites for high toughness (top row) and strength (bottom row). Reprinted from Ref. [68], Copyright 2018, with permission from Elsevier. (*b*) Hierarchical design units (left) and optimized designs for high toughness (right). Reproduced (adapted) from Ref. [26] with permission from the Royal Society of Chemistry. (*c*) Predictions of stress and strain fields of composites with pixel-level material distributions using conditional GAN. Reproduced from Ref. [70], Copyright 2021, The Authors, published by AAAS. (*d*) Inverse identification of material distributions based on boundary displacements using physics-informed ML. Reproduced from [71], Copyright 2022, The Authors, published by AAAS. (e) VAE enabled low-dimensional, highly structured latent space of microstructures, which allows for the generation of diverse architecture families with gradually varying geometries and stiffness. Reprinted from Ref. [72], Copyright 2020, with permission from Elsevier. (*f*) Forward and inverse ML-enabled two-way structure–property mapping, where the training of inverse NN is supervised by the pretrained forward NN. Reproduced from Ref. [73], Copyright 2020, The Authors, published by Springer Nature.

structural topologies (a form of heterogeneous materials) is a typical inverse problem in TO. A variety of ML models such as GAN [77] and CNN [78] have been developed for TO tasks. These works are not elaborated on here, and the readers may refer to a recent review [79].

2.2 Stress and Strain Fields

2.2.1 Forward Prediction and Material-Distribution Design. Apart from macroscopic mechanical properties, the physical fields (e.g., stress and strain fields) are often of interest. One associated forward problem is the prediction of stress or strain fields in a given structure. Nie et al. [80] proposed a CNN model that can predict the stress fields of cantilever structures with moderately arbitrary topologies and loads. Buehler and coworkers [70] developed a conditional GAN-based ML approach, which can predict the stress and strain fields of composites with pixel-level material distribution, as shown in Fig. 2(*c*). The model also demonstrated the applicability to different component shapes, boundary conditions, and geometric hierarchies. Later on, they further extended this approach for the complete strain and stress tensor predictions and demonstrated enhanced model generalization by enriching the training datasets with different hierarchies and constituent ratios [81].

The inverse problem, which is manifested as various specific tasks and applications in different fields, has attracted significant interest. In the context of 3D printing, the goal is to design the material property distribution to achieve the target physical field under external loads. Montgomery et al. [27] managed to realize locally tunable anisotropy by using grayscale DLP printed microstructural patterned units, where the CNN model was employed for the macroscale design of the property field when target strain fields were given.

2.2.2 Material Characterization in Experimental Mechanics. In experimental mechanics [52,53], the inverse problem holds particular significance for the material characterization or elastography, i.e., to identify the mechanical property field based on a measured deformation field. Various ML methods have been developed for this problem. Although it differs from the design problem in 3D/4D printing, the underlying objective for both problems is to establish a mapping from deformation to property, suggesting that ML methodologies developed for one might be adapted for the other. Therefore, we briefly discuss the ML strategies used in the material characterization here.

Physics-informed neural networks (PINN), pioneered by Karniadakis and coworkers [82], have made significant advancements. PINN has been applied to various systems governed by partial differential equations (PDEs), both for forward and for inverse problems. Specifically, Zhang et al. [83] implemented a PINN to determine the modulus field of nonhomogeneous hyperelastic materials subjected to external loads, based on the applied boundary displacement data. Later on, they expanded the approach to materials with heterogeneous inclusions or defects [71]. Using PINN, they were able to identify both the geometry (or topology) and elastic properties of the inclusions (Fig. 2(*d*)), which was demonstrated for materials with various constitutive behaviors, possibly with large deformations or plasticity. Moreover, a similar PINN approach was recently proposed by Mowlavi et al. [84], who demonstrated the identification of inclusions with unknown numbers, various properties, and irregular shapes. In addition to the works above, other PINN methods have been proposed to identify nonhomogeneous mechanical properties using full-field experimental data [85–89]. One of the major advantages of PINN is that it can integrate physical laws and data in the loss function, and thus requires no or a small amount of data in many cases. Additionally, while PINN does not outperform conventional methods such as finite element (FE) simulations for forward problems [90], it demonstrates superior performance for many inverse problems [53].

In essence, PINN represents an optimization method leveraging the strong expressivity of deep neural networks. Despite its strength, this optimization nature implies that a fresh optimization run is required for each unique deformation field, making individual tasks time-consuming. SL, although requiring a large amount of labeled data, can function much faster once the training is complete and thus has also been employed for inverse material characterization tasks. For example, Liu et al. [91] developed an ML model that combines discrete cosine transform (DCT) and CNN for accurate modulus field identification. The DCT was used to transform data into the frequency domain, thereby achieving dimensionality reduction and noise filtering. The CNN was then utilized to learn the inverse mapping of frequency data from the strain to the modulus field. This demonstrates the importance of dimensionality reduction in SL tasks when the design or property space is huge.

2.3 Mechanical Metamaterials. Mechanical metamaterials, or architected materials, represent a broad class of engineered structures whose properties are determined more by their geometric configurations than by the constituent materials. They often involve intricate microstructural units (or architectures), making them highly amenable to fabrication via 3D printing. Such microstructures can yield exotic properties, such as tailorable anisotropy, unusual stress–strain curves, negative Poisson's ratios, and tunable acoustic properties. Therefore, the inverse microstructural design for desired properties is a significant facet in the 3D/4D printing design.

2.3.1 Anisotropic Elasticity by Generative Models. In the design of mechanical metamaterials, an important objective is to achieve the desired, often anisotropic, stiffness tensor. Here, the associated forward problem, i.e., predicting the homogenized elastic stiffness tensor of an architecture (often referred to as homogenization), is typically more tractable using supervised ML models. However, the inverse problem presents a significant challenge as it is ill-posed due to the infinite-dimensional geometric design space and the one-to-many mapping nature from properties to structures. To tackle the inverse problem, deep generative models have been employed to spawn new complex architected designs. For example, Zhao and coworkers [92] developed a GAN model that learns microstructural features from the enormous database they built. This model was then used to generate a myriad of isotropic-elastic architectures that approach the Hashin-Shtrikman (HS) upper bounds under a wide range of porosity values (from 0.05 to 0.75). Additionally, Li and coworkers [93] used a GAN to generate new 3D lattice structures whose compression strength was evaluated using a forward GP regressor [94], thus discovering novel lattice architectures with high compression strength. Moreover, they utilized a GP regressor for finding novel 2D lattices with high recovery stress [95].

Note that the design objective of these GAN-aided tasks is relatively limited, e.g., to extremizing a specific property. When we desire the target property to vary within a range, e.g., designing functionally graded metamaterials with spatially varying properties and microstructures, the problem becomes considerably more challenging. To tackle this challenge, Chen and coworkers [72] utilized the VAE to aid the design process (Fig. 2(*e*)). After a large database is built, the encoder within the VAE can compress the microstructure information into a low-dimensional, highly structured latent space, from which the initial structure can be restored by the decoder. A forward predictor (i.e., regressor) was further employed to learn the relationship between the latent variables and the stiffness. As shown in Fig. 2(*e*), by continuously sampling points in the latent space, they generated diverse architecture families with gradually varying geometries and stiffness. This, in conjunction with conventional macroscale TO, enabled the multiscale design of functionally graded metamaterials that achieve target shape changes. Later on, Chen and coworkers [96] further utilized the same approach for the design of metamaterial-based mechanical cloaks. In addition to VAE, they employed latent variable GP to obtain a latent space for the designs of 2D and 3D lattice metamaterials [97].

Moreover, EA may be seen as a form of generative modeling, which often requires high computational cost due to its stochastic search nature. Yu et al. [98] recently combined EA with a forward ML model to design lattice-based artificial spinal discs with desired anisotropic behaviors.

2.3.2 Anisotropic Elasticity by a Forward Machine Learning-Supervised Inverse Machine Learning Model. Alternatively, Kochmann and coworkers [73] proposed a general inverse design framework that ingeniously exploits a forward ML model to supervise an inverse ML model and applied it to the spinodoid metamaterials. Figure 2(*f*) illustrates the concept of this approach. The forward ML model, which takes the design parameters as input to predict the stiffness (property), is pretrained using labeled data and then leveraged to train the inverse model through the following procedure. The inverse model takes the target property as input and yields a trial design, which is fed into the forward model to predict the trial property. The inverse ML model is trained by minimizing the discrepancy between the predicted and target properties. Once trained, the inverse model can instantaneously generate the optimized designs on demand while the forward and inverse models together also provide a computationally efficient two-way structure–property mapping. Moreover, their approach enables the design of spatially varying architectures for functional grading. Later on, they extended this design framework to truss (or lattice) metamaterials by incorporating an appropriate design parameterization [99], as well as to the pore growth-based cellular metamaterials [100]. More recently, they incorporated the forward ML model into gradient-based multiscale TO, where the ML allows for rapid forward homogenization for given microstructures and efficient computation of gradients via automatic differentiation (AD), enabling the accelerated multiscale TO of functionally graded spinodoid metamaterials [101].

2.3.3 Stress–Strain Response. Owing to their unique microstructures, mechanical metamaterials often exhibit unusual stress–strain curves under external loads. The rational design of these structures, aimed at achieving diverse target load-deformation responses, holds significant engineering values. Given the vast geometric design space, ML has been exploited to accelerate the inverse design process. For instance, Wang et al. [102] combined an NN forward model and an EA to design novel central-symmetry, shell-based metamaterials with various target compressive stress–strain curves, such as strain hardening and softening. Note that a large number of data points are needed to well represent a stress–strain curve, which implies high data dimensionality and can impair network performance. Employing multiple NNs can improve performance while increasing computational cost [102].

This issue is addressed in an alternative study with a different metamaterial (i.e., a kirigami metamaterial), where Deng et al. [103] utilized PCA to condense the stress–strain data, obtaining their principal components. They then trained an NN to directly learn the relationship between the geometric design parameters and the resulting principal components, which achieves high prediction accuracy. Combining NN with an evolution strategy (a class of EA), they achieved an effective inverse design. Notably, they also attempted to use an inverse NN to map from response to design; the results showed that an inverse NN does not perform well due to the ill-posed nature of the inverse problem. Yet, a recent work [104] with lattice metamaterials demonstrated the applicability of a forward ML-supervised inverse ML (similar to that described in Sec. 2.3.2) in designing stress–strain curves, where the appropriately tailored design space is important. Moreover, the video-denoising diffusion model has been used to design the stress–strain response of cellular metamaterials, which can also concurrently predict the full-field internal stress distribution [105]. Additionally, Bayesian ML has been explored in the design of super-compressible metamaterial blocks [106].

In addition to the mechanical response mentioned earlier, other physical properties of metamaterials, including acoustic and optical properties, have attracted significant interest and inspired studies utilizing ML methods [107–110]. We will not elaborate on these here but refer the readers to a recent review [111].

2.4 Active Shape-Change Response by 4D Printing. Integrating 3D printing with active materials (or stimuli-responsive materials) enables the emerging 4D printing technique [8]. The ability of multimaterial 3D printing to spatially control the mechanical properties of structures further offers a vast design space. In general, the 4D printing concept is not limited to shape changes but is also applicable to property or functionality changes. In this section, we mainly discuss works using ML for designing shape-change responses in 4D printing, possibly involving general active material systems. Generally speaking, design for shape change could be more challenging than that for mechanical properties such as stiffness and toughness, as high-dimensional data are needed to fully describe a shape change.

2.4.1 Finite Element—Evolutionary Algorithm Approach. To exploit the large design space offered by multimaterial 3D printing, the computational design integrating mechanical simulations and optimizations has become a highly capable tool. For example, the gradient-based TO has made great progress [40–44,46–48], yet it may suffer from low design efficiency and high numerical complexity when geometric and material nonlinearities are involved. Alternatively, gradient-free optimization algorithms such as EA have also achieved great success. For example, Hamel et al. [112] employed the FE and EA (FE-EA) for the inverse design of active composite (AC) beams with voxel-level material distributions. The approach was later extended to magneto-AC beams by Wu et al. [113], who also developed a voxel-level encoding approach in the DIW 3D printing method. Athinarayanarao et al. [114] used an FE-EA approach to design AC beams integrated with topological void voxels. The FE-EA approach is time-consuming and cannot deal with very complicated target shapes. This is because the EA typically requires numerous forward FE simulations to explore a large design space, thus suffering from high computational cost.

To reduce the computational cost, researchers have developed forward reduced order models (ROMs) to speed up evolutionary designs for different material systems, such as 3D voxel ACs [115,116] and magneto-AC beams [117,118]. Yet, faster forward models, preferably capable of handling vast amounts of data, are still highly desired to enable more efficient inverse designs. As such, the ML approach is particularly suited for delivering ultrafast, massive predictions and has been extensively exploited to address the inverse design problem.

2.4.2 Integrated Forward Machine Learning and Optimization Algorithms. One common approach is to use ML as a forward predictive model and subsequently integrate it with optimization algorithms for the inverse design. In this case, it is crucial to select an appropriate network architecture based on the specific design problem (active material systems, target response, etc.). For AC beams, Zhang et al. [119] applied multiple ML models to the forward prediction problem and found that CNN performed best. Later on, Sun et al. [120] found that the RNN is particularly suited for the beam problem as it inherently preserves a sequential data dependency similar to that arises from the beam deformation (Fig. 3(*a*)). The RNN thus demonstrated remarkably high accuracy in the forward shape prediction based on material distributions, which then empowered EA to achieve highly efficient inverse designs of complicated, even hand-drawn, target shapes. For another AC system, magneto-mechanical metamaterials, Ma et al. [121] ingeniously encoded the magnetization distribution into a 2D array and utilized a deep residual network (ResNet) model to learn the relationship between magnetization distribution and active strain (Fig. 3(*b*)). They further demonstrated the ResNet-empowered discrete artificial bee colony (DABC) algorithm can rapidly achieve inverse designs for various target active strains and Poisson's ratios. In addition, ML has been used for designing shape changes of auxetic metamaterials with hierarchical pattern distributions [124] and for predicting the bending angle of soft pneumatic robots given geometric parameters [125].

2.4.3 Inverse Machine Learning Approaches. One alternative approach is to train an inverse ML model that maps from the target response to the optimized design. For example, for inflatable composite membranes, Forte et al. [122] successfully utilized an inverse NN to learn the mapping from 3D target inflated shapes to the optimized 2D pixel-level material distributions (Fig. 3(*c*)). Similarly, for buckling mesosurfaces, Zhang and coworkers [123] trained an inverse NN to directly predict the optimized microlattice precursor configurations needed to realize complex target surfaces upon buckling (Fig. 3(*d*)). More recently, they applied a similar strategy for the inverse design of buckling frame structures that can morph into complex target shapes [126]. Note that these inverse ML models were all trained to learn the inverse mapping

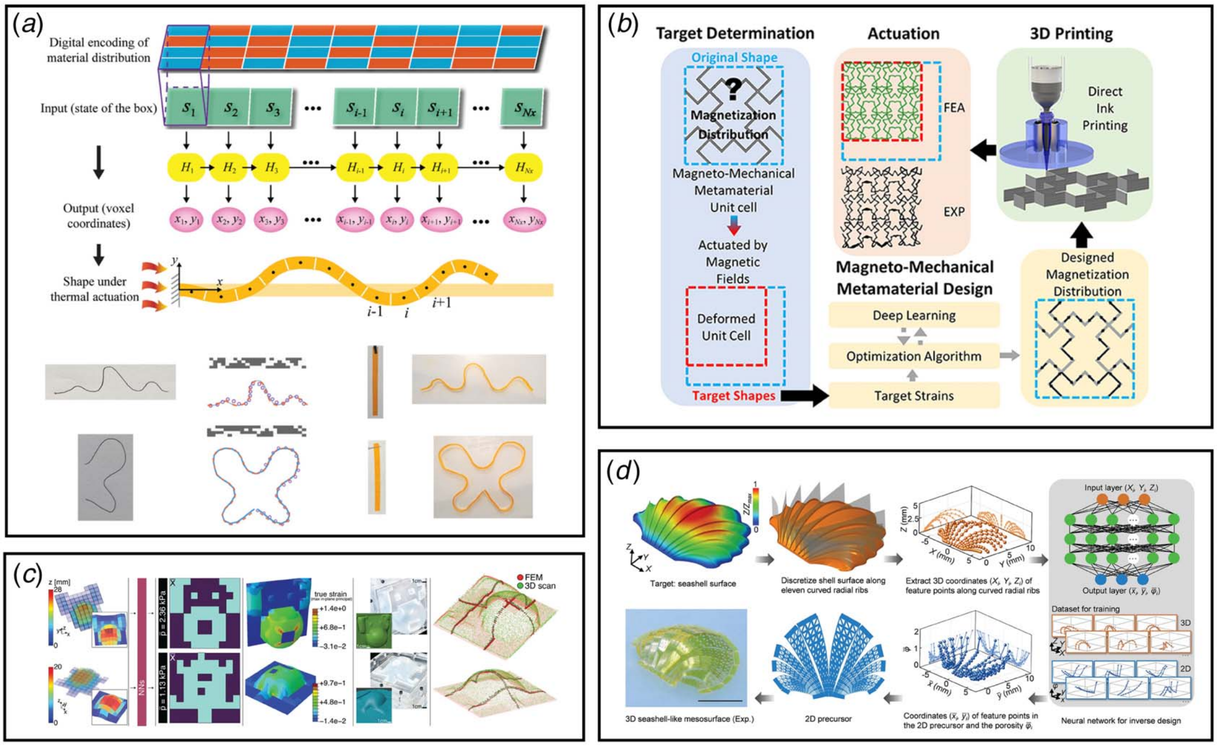

Fig. 3 Applications of ML in various active material systems for designing active shape-change responses. (*a*) Forward predictions using RNN-based ML and inverse design using ML-EA for 4D-printed AC structures. Reproduced (adapted) with permission from [120]. Copyright 2021, John Wiley and Sons. (*b*) Forward predictions using ResNet and inverse design using a ResNet-empowered DABC algorithm for 4D-printed magneto-mechanical metamaterials. Reprinted with permission from Ref. [121]. Copyright 2022 American Chemical Society. (*c*) Inverse design of inflatable composite membranes using an inverse NN. Reproduced with permission from Ref. [122]. Copyright 2021, John Wiley and Sons. (*d*) Inverse design of buckling mesosurfaces using an inverse NN [123]. Reprinted with permission from AAAS.

directly from the data. Despite their successes, such models may struggle with complex inverse problems where multiple distinct designs can produce very similar responses (thus causing a one-to-many issue that can be harmful to the training), as exemplified in the design of metamaterials [103]. In this case, the use of forward ML to supervise an inverse ML model [73] can facilitate learning the inverse map, as discussed in Sec. 2.3.2. Espinosa and coworkers [127] utilized this approach to program the shape changes of kirigami metamaterials upon tension-induced buckling.

3 Perspective

It is typically more tractable to learn the forward mapping from designs to responses given labeled data. However, the inverse problem is challenging as it is ill-posed due to the large, often infinite-dimensional, design space and the one-to-many mapping nature from responses to designs. Moreover, in many design tasks, instead of simply optimizing or extremizing a single property, the target response is desired to vary within a range, such as achieving the various target mechanical properties or attaining different target shape transformations under external stimuli. This scenario makes the inverse design more challenging, particularly when the target response involves high-dimensional data, such as the shape-change response. ML holds significant promise in tackling these challenges. In the following, we briefly summarize existing and potential strategies for the effective application of ML in 3D/4D printing designs (Fig. 4).

In inverse design, accurate forward prediction is crucial, and depending on the specific problem, it may require varying amounts of data. As the design space is typically huge, using some data dimensionality reduction methods, such as PCA, DCT, and autoencoder (AE), to pre-compress the data often facilitates learning and improves performance. Additionally, observing the specific problem to select an appropriate network architecture is important. With an efficient forward ML (F-ML) model in place, several strategies exist for optimization.

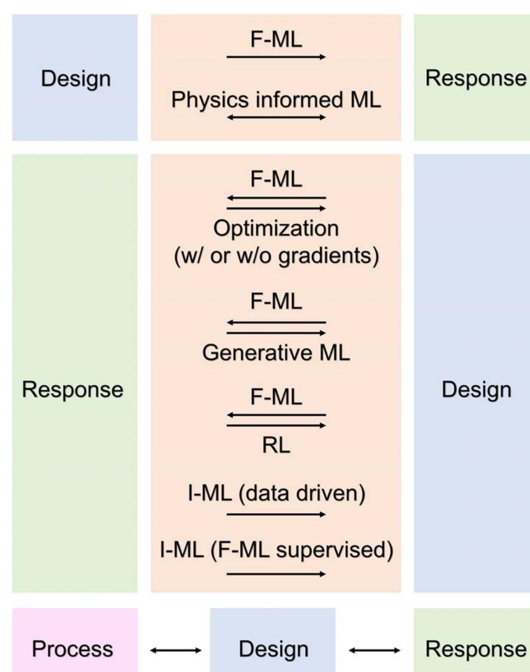

Fig. 4 Overview of ML strategies for designs in 3D/4D printing

First, an F-ML can be combined with an optimization algorithm, either gradient-based or gradient-free, for the inverse design. Compared to conventional computational methods, the high speed of ML allows for accelerated design with any optimization algorithms, as they all involve the forward prediction steps. Additionally, the automatic differentiability of F-ML allows for efficient computation of gradients (or sensitivities) and thus can significantly accelerate gradient-based optimizations.

Second, methods that utilize generative models like VAE [72] or GAN [70,128] to generate new designs and use an F-ML for screening may be employed. Specifically, VAE can be used to create a continuous, structured latent space, and in this case, the F-ML can learn the mapping from the latent variables to the property. Note that EA may also be seen as a form of generative modeling.

Third, integrated F-ML and RL may be used for the inverse design. Previous studies have employed RL for the toughness maximization of 3D-printed composites [76] and the compliance minimization of structural topologies [129]. In these works, the FE was utilized for the reward evaluation during the RL training, which is computationally expensive. Integrating pretrained F-ML with RL could significantly improve design efficiency, rendering RL more feasible for large-scale problems.

Furthermore, methods based on inverse ML (I-ML) can be used, which may or may not need F-ML depending on the specific training strategy for the I-ML. One strategy is to directly train the inverse model using labeled data, which can be effective at times [91,122] but often fails for complex inverse problems [103,130] due to the ill-definition (i.e., one-to-many mapping). An alternative strategy leverages the F-ML to train the I-ML (i.e., F-ML-supervised I-ML) [73]. In this case, the I-ML takes the target property as input and yields a trial design, which is fed into the F-ML to predict the trial property. The training of the inverse ML model is done by minimizing the difference between the predicted and target properties. Moreover, the I-ML training may be supervised by other differentiable forward models such as ROMs, not necessarily F-ML. For all strategies earlier, once the training is complete, the I-ML can promptly generate the optimized designs.

To delve even further into the perspectives and, more specifically, to leverage the benefits of ML while ensuring a complete understanding, there is a strategic need to integrate materials/design informatics and ML for scientists [131–133]. This trend of merging symbolic AI and ML is commonly referred to as neuro-symbolic integration. It entails constructing a comprehensive knowledge/database enhanced with computational procedures to discover innovative materials and structures. Symbolic logic representations can then be used in ML to incorporate background knowledge in learning models and algorithms. This approach ensures transparency to humans, deductive reasoning, the integration of expert knowledge, and structured generalization, particularly in scenarios with limited data where physics is essential [134,135]. This symbolic AI layer proves valuable for working with small datasets and/or providing rationale in quantitative investigations involving extensive data generated from high-throughput computational materials design.

Beyond achieving material or structural designs with optimized responses, the reliable and accurate printing of intended designs is also crucial. This involves issues such as design optimizations considering manufacturability/printability, printing parameter refinement, quality monitoring and control, and material design and discovery. Additionally, integrated design for the process–structure–property mapping may be important [136]. Using DLP as an example, the desired voxel-level material distributions may deviate significantly from the actual printing, especially for small-sized objects, due to factors such as light penetration, uneven light distribution, and species reaction-diffusion [27,137]. In this case, refining printing parameters (e.g., light field distribution) for appropriate compensations poses a multiphysics inverse problem, which may also be addressed using ML strategies outlined above.

In conclusion, this perspective paper highlights the rapidly growing role of ML in addressing complex inverse design problems in 3D/4D printing. First, we provide an overview of common forward and inverse problems, relevant types of structures, and design space and responses in 3D/4D printing. Next, by reviewing recent works that employ a variety of ML approaches, we provide an in-depth discussion on how ML can be harnessed to design printed structures with specific mechanical responses, from structural properties to load-displacement responses, physical fields, and active shape changes. Finally, after discussing the challenges, we highlight the existing ML approaches and discuss their potential extensions. Broader design problems in the field of 3D/4D printing are further discussed. Despite existing challenges, the integration of ML into 3D/4D printing design has immense potential to revolutionize the field. Our work aims to serve as a foundational guide, offering critical insights for researchers and practitioners looking to leverage ML for efficient and intelligent designs in additive manufacturing.

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Conflict of Interest

There are no conflicts of interest.

Data Availability Statement

No data, models, or code were generated or used for this paper.

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