Optimizing stimuli-based 4D printed structures: a paradigm shift in programmable material response

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ABSTRACT

This paper introduces a methodology for optimizing 4D printing design through the integration of Residual Neural Network (ResNet) and Genetic Algorithms (GA). Departing from traditional forward design approaches, our inverse design methodology addresses both the forward prediction and inverse optimization problems. ResNet efficiently predicts the performance of 4D-printed parts given their design, while GA optimizes material allocation and stimuli distribution to achieve desired configurations. The ResNet model exhibits high accuracy, converging to a small error (10^{-3}), as validated across diverse cases. The GA demonstrates effectiveness in achieving optimal or near-optimal solutions, illustrated through case studies shaping parts into a parabola and a sinusoid. Experimental results align with optimized and simulated outcomes, showcasing the practical applicability of our approach in 4D printing design optimization.

Keywords: 4D printing, inverse design, additive manufacturing, machine learning, residual neural network, genetic algorithm

1. INTRODUCTION

In recent years, the field of additive manufacturing has witnessed a groundbreaking evolution with the emergence of 4D printing—a revolutionary approach that introduces the dimension of time into the fabrication process.[1–5] The predominant approach in current 4D printing research revolves around a forward design methodology,[6–8] that is, the process of creating a 4D printed part begins with the initial design of a prototype. Subsequently, this design is physically realized through the 4D printing process, and the resulting part is evaluated to assess its alignment with the intended requirements. If the printed part fails to meet the specified criteria or if there is room for improvement, the designer iteratively revisits the drawing board, making adjustments to the design, and the cycle repeats. This methodology is commonly referred to as the empirical method or trial and error.

One of the primary challenges associated with the empirical method is the resource-intensive nature of the iterative process.[9] Each cycle of design, printing, and evaluation demands time, materials, and effort. As a result, the overall development timeline may be prolonged, hindering the efficiency of the design optimization process. Additionally, the empirical method may lead to a substantial waste of materials as unsuccessful iterations contribute to the accumulation of discarded prototypes.[10] Moreover, the forward design methodology

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may encounter difficulties in predicting the behavior of complex 4D printed structures accurately. The intricate interdependencies between stimuli and materials often introduce non-linearities that can be challenging to anticipate through conventional design approaches. This unpredictability may necessitate numerous iterations before achieving the desired outcome, contributing to an extended and sometimes unpredictable design timeline.

In contrast to the forward design methodology, our research paper introduces an inverse design approach by incorporating Residual Neural Network (ResNet) and Genetic Algorithms (GA) into the 4D printing design optimization process. ResNet addresses the forward prediction problem in 4D printing design—given the part design, it predicts the performance of the designed part. While finite element analysis is a common method for the forward problem, it tends to be time-consuming, especially when dealing with a large number of cases for dealing with the inverse problem. In contrast, machine learning, facilitated by ResNet, offers a more efficient alternative. GA is employed to tackle the inverse optimization problem in 4D printing design—given the desired configuration, it determines how to design the allocation of stimuli or the distribution of materials so that the inverse-designed part aligns with the desired configuration. This dual approach aims to transcend the limitations of the empirical method, providing a more systematic and efficient means of achieving desired configurations in 4D printed structures. The integration of machine learning and evolutionary principles in our methodology enhances the predictive capabilities of the design process, significantly reducing reliance on extensive trial and error. This strategic combination enables a more intelligent and adaptive approach to 4D printing design optimization, marking a departure from traditional empirical methods and opening new avenues for efficient and precise structural configuration attainment.

The current research status of inverse design in 4D printing is in the preliminary stage of development. Notable studies, such as Hamel et al.[11]'s machine-learning-based approach, emphasize the intricate design of active composite structures through the integration of multimaterial 3D printing and evolutionary algorithms. Similarly, Athinarayanarao et al.[12] focus on computational design for topology-optimized multi-material active composites, employing finite element analysis-based evolutionary algorithms and topology optimization to address the inverse design problem. Sun et al.[13] contribute a novel methodology by combining machine learning and evolutionary algorithms for 4D-printed active composite structures, demonstrating efficiency in achieving multiple target shapes. Additionally, Zhao et al.[14]'s work explores the application of machine learning and evolutionary algorithms in optimizing grayscale distribution for grayscale digital light processing (DLP) 3D printing blocks. In this context, our paper introduces an innovative methodology, departing from traditional finite element analysis, by integrating Residual Neural Network and Genetic Algorithms. This new approach promises a more systematic and efficient means of achieving desired configurations in 4D printed structures, overcoming the time-consuming nature of existing forward prediction methods and paving the way for advancements in 4D printing design.

The structure of the remaining sections in this paper is outlined as follows: In Section 2, the structure and the materials used in this paper will be presented. Section 3 will provide a detailed demonstration of the forward prediction methodology utilizing ResNet. Following that, Section 4 will delve into the discussion of the inverse optimization method employing Genetic Algorithms. In Section 5, we will present the outcomes of both inverse design and experimental results, specifically focusing on two distinct cases—the parabola and sinusoid shape. Finally, Section 6 will encapsulate the conclusions drawn from our study and initiate a discussion on potential future works in the realm of 4D printing design optimization.

2. STRUCTURE DESIGN AND MATERIAL SELECTION

Compared to 3D printing, 4D printing involves the manufacturing of materials and structures that can undergo dynamic transformations over time in response to external stimuli, including heat,[15–17] light,[18–21] electric fields,[22] magnetic fields,[23] and moisture.[24–26] The mechanics of 4D printing are rooted in the properties of smart materials, which have the ability to change their shape, structure, or properties when subjected to specific environmental triggers. For 4D printing of digital materials, the main power that drives the shape change of parted parts lies in the material property difference of the digital materials.[27] In our exploration of 4D printing with digital materials, we distinguish these two digital materials: the active material, characterized by its large deformation in response to applied stimuli, and the passive material, exhibiting comparatively minimal deformation under the same conditions. As shown in Figure 1, the red pixel represents the active materials and the

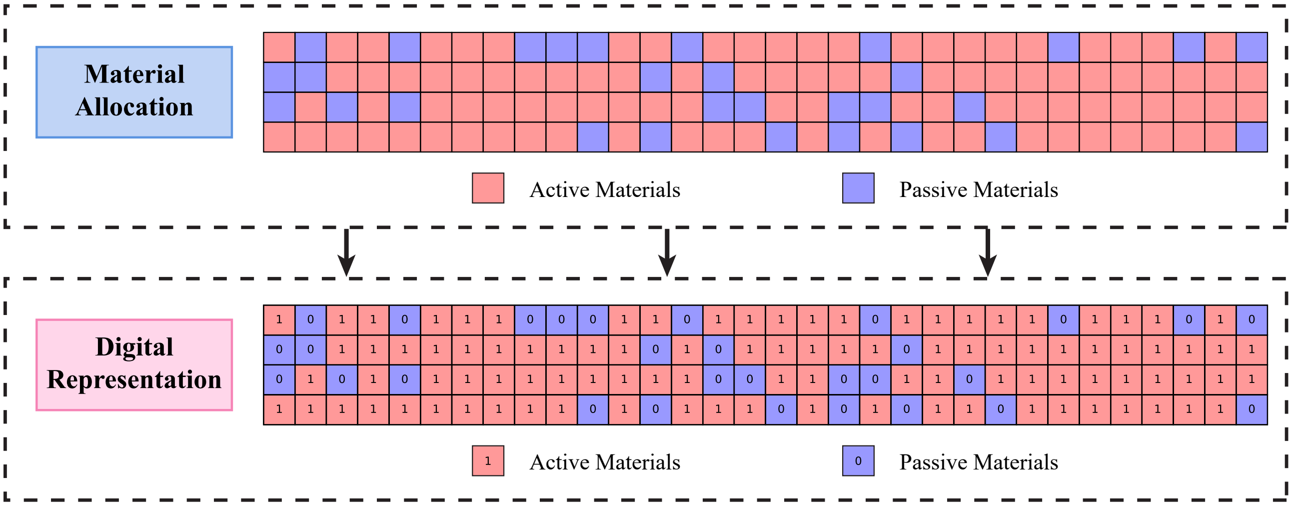

Figure 1. The demonstration of digital representation of active and passive materials.

blue pixel represents the passive materials. As input to the machine learning of material allocation, we use 1 for active materials and 0 for passive materials, which is demonstrated in Figure 1 as digital representation. The allocation of the active materials and passive materials will cause different behavior of 4D printed parts.

In the context of our research, we focus on analyzing a specific configuration consisting of 4×32 pixels. Each pixel is characterized by dimensions of 5 mm $\times$ 5 mm. To demonstrate the principles discussed in this paper, we selected shape memory polymer (SMP) obtained material property data from SMP Technology in Japan as the active material. Concurrently, TPU is employed as the passive material in our study. This particular setup serves as an illustrative example for our comprehensive analysis of the 4D printing inverse design and the influence of material properties on shape transformations.

3. FORWARD PREDICTION METHODS FOR 4D PRINTING

In this section, we will present the Residual Neural Network model we designed for the forward prediction of 4D printing, which is demonstrated in Figure 2. This ResNet model is utilized to predict the deformation of the 4D-printed parts with the specific material allocation. ResNet is introduced to tackle challenges like vanishing gradients and degradation in traditional deep networks.[28] ResNet addresses these issues through skip connections, enabling the efficient flow of information and facilitating the training of extremely deep networks. By introducing residual blocks and identity mapping, ResNet learns to preserve information throughout the network, allowing for the capture of intricate features. This not only overcomes the limitations of depth but also accelerates convergence, making ResNet computationally efficient. Their versatility is highlighted by superior generalization capabilities and performance across various tasks, outshining Convolutional Neural Networks (CNNs) in spatial hierarchies and Recurrent Neural Networks (RNNs) in sequential data. ResNet's impact lies in its ability to seamlessly integrate spatial and sequential domain features, making them a fundamental and widely adopted architecture in deep learning.

The data preprocessing procedure is devised to normalize the input and output data. The input data, representing active (1) and passive (0) allocation matrices, is normalized by the equation $x_n = (x - 0.5)/0.5$, where x is the input data and x_n is normalized input data. This equation converts the original 0, 1 to -1, 1. On the other hand, the output data is normalized based on the mean and standard deviation, which can be represented by $y_n = (y - y_{mean})/y_{std}$, where y is the output data, y_n is the normalized output data, and y_{mean} and y_{std} represents the mean and the standard deviation of all output data, respectively. This normalization procedure ensures that the output dataset attains a mean of 0 and a standard deviation of 1. The normalized data is then organized into training and validation sets for model training. The percentages of the training and validation datasets are 80% and 20%, respectively. The training dataset is used to train the machine learning

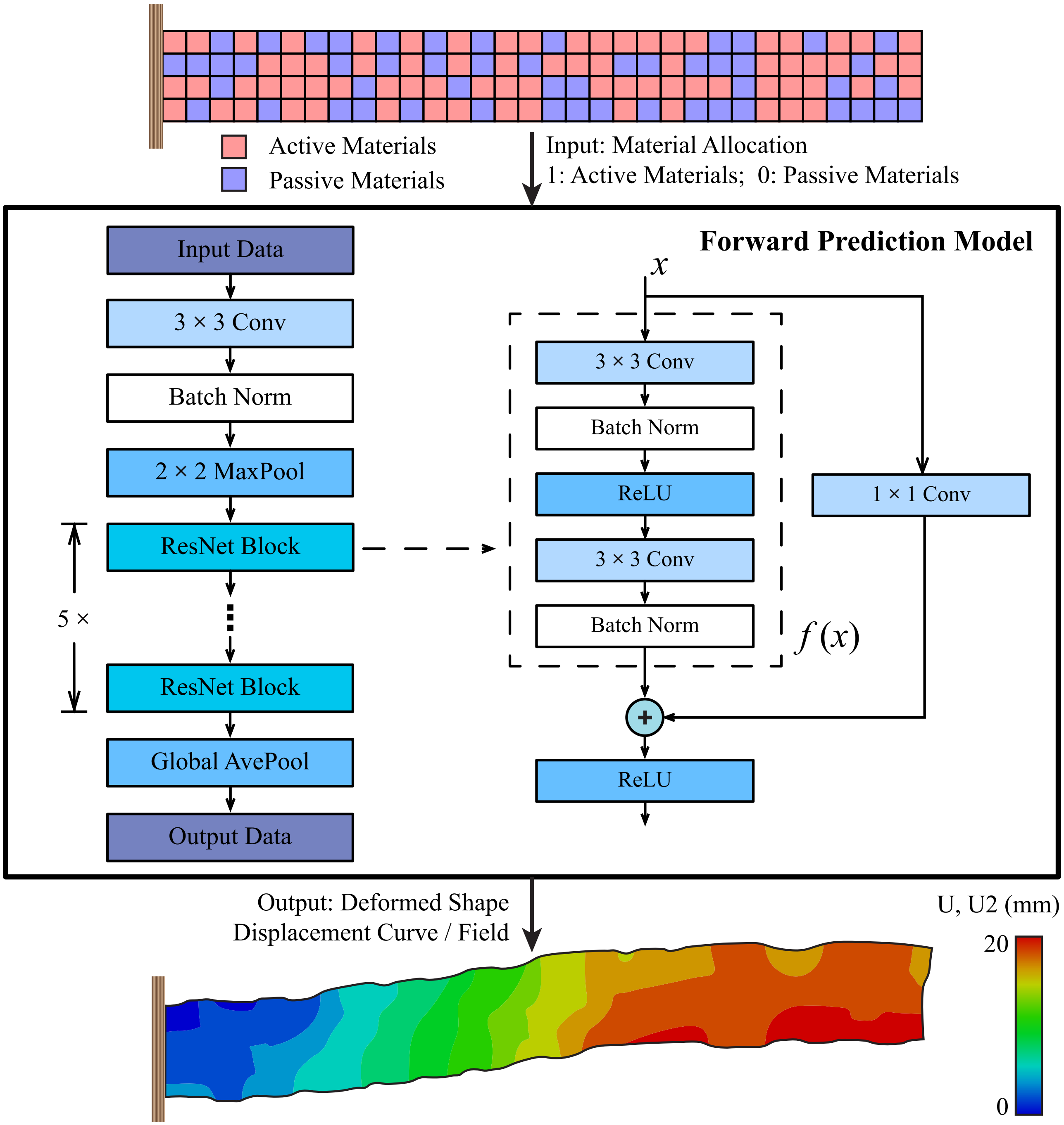

Figure 2. Forward prediction model constructed by ResNet to predict the deformation based on the material allocation.

model. During the training process, the model learns the patterns and relationships within the input data and its corresponding output. The goal is to enable the model to make accurate predictions or classifications on new, unseen data. Meanwhile, the validation dataset is used to assess the performance of the model during training and to make decisions about hyperparameters or the overall architecture of the model. It serves as an independent dataset that the model has not seen during training.

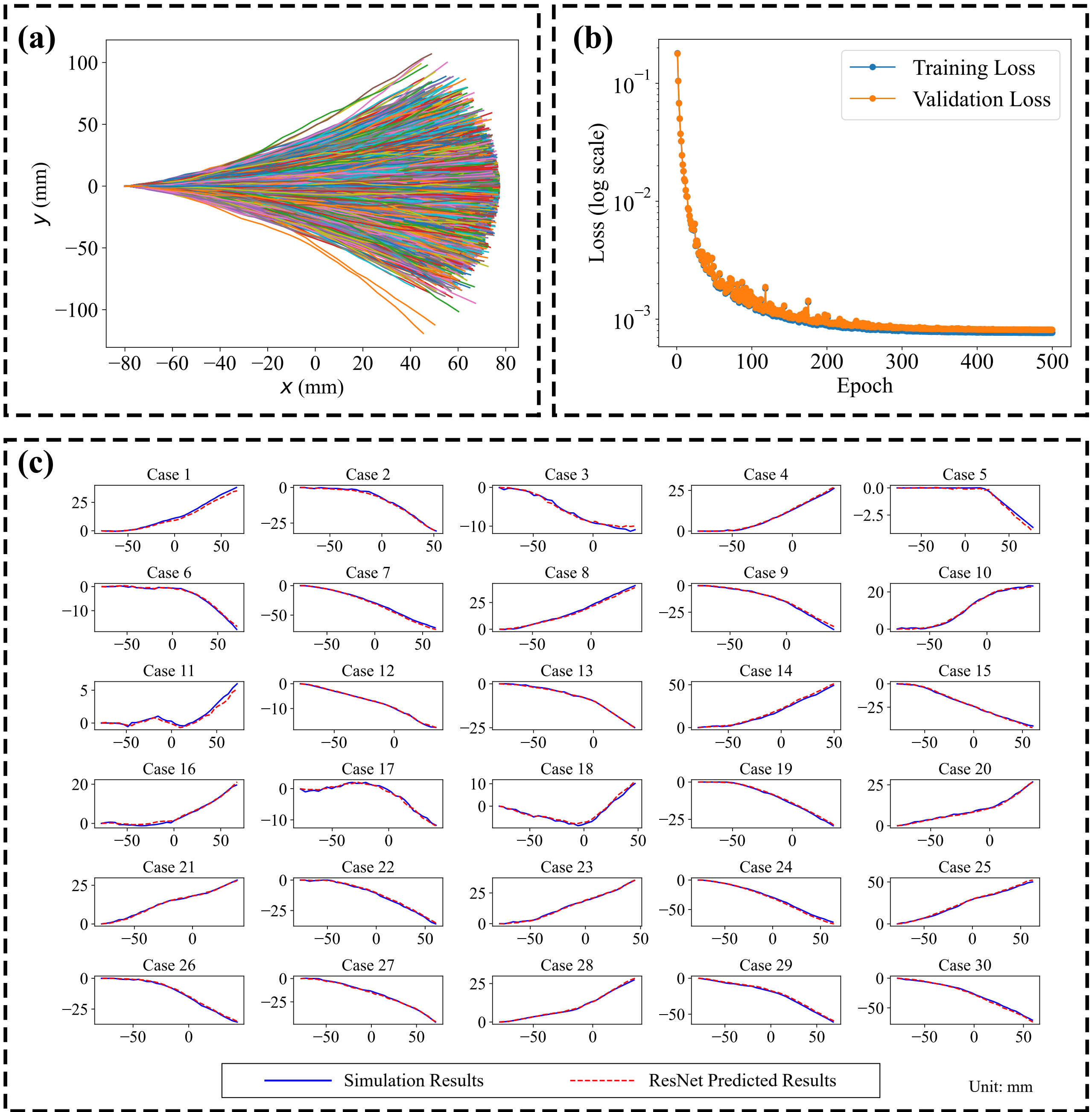

Figure 3. The performance of forward prediction model (ResNet). (a). All the datasets (20,000) for training and validation. (b). The training loss and validation loss for the forward prediction model. (c). The comparison between simulation results and ResNet predicted results for 30 cases.

The architecture of the ResNet model involves convolution layers, max-pooling, and residual blocks, which is illustrated in Figure 2. The input layer consists of a convolution layer with 4 filters and a $(3, 3)$ kernel size, followed by max-pooling. Five residual blocks, each with convolution layers employing 8 filters, contribute to the model's depth. The output layer is a fully connected layer with a linear activation function, shaping the model's output to the desired form.

This ResNet model we designed involves several hyperparameters. The learning rate dictates the step size in adjusting the model weights during optimization, with a value set at 0.0005. The batch size parameter specifies the number of samples processed in each mini-batch during training, set to 50. Additionally, the max epochs parameter defines the maximum number of training iterations, capped at 500, while the loop decay factor determines the rate at which the learning rate diminishes over epochs, which is set to 0.6 per 25 epochs.

The training loops facilitate the model's learning process. The model is compiled using the Adam optimizer and mean squared error as the loss function. The training loop iterates over epochs, fitting the model to the training data and evaluating both training and validation losses. Additionally, early stopping is employed to halt training if the validation loss fails to improve for a set number of consecutive epochs.

The performance of the forward prediction model is depicted in Figure 3. A dataset comprising $20,000$ instances of both input and output data is utilized to train and validate the ResNet model. In Figure 3(a), the deformation of 4D-printed parts along the horizontal central lines is illustrated for all $20,000$ cases. Figure 3(b) presents the training and validation loss across 500 epochs. Notably, both the training and validation losses converge to a minimal error (10^{-3}), underscoring the efficacy of the constructed forward prediction model. This observation is further affirmed in Figure 3(c), where simulation results and ResNet predictions for 30 cases are compared. Remarkably, the ResNet predicted results closely align with the simulation results for all 30 cases, demonstrating the model's capability to accurately predict the deformation of 4D-printed parts.

4. INVERSE OPTIMIZATION METHODS FOR 4D PRINTING

In this section, we will demonstrate the Genetic Algorithm model designed for the inverse optimization of 4D printing. Rooted in evolutionary biology, GAs emulate the process of natural selection to evolve solutions for complex problems.[29] A population of potential solutions undergoes iterative generations, where individuals are encoded as chromosomes, and their fitness is evaluated based on their ability to solve the given problem. Through mechanisms like crossover and mutation, genetic algorithms mimic genetic recombination and variation to produce new candidate solutions. The survival of the fittest individuals influences the evolution of the population over successive generations, ultimately converging toward optimal or near-optimal solutions.

The genetic algorithm workflow for 4D printing design optimization unfolds in several iterative steps, each contributing to the evolution of the population toward increasingly optimal solutions. The process begins with the generation of an initial population comprising 5,000 individuals, each representing a potential solution for the material allocation and stimuli distribution in 4D printing. These solutions are randomly generated, reflecting diverse configurations for the 4D-printed structures.

Subsequently, each individual in the initial population undergoes evaluation through a fitness function, which quantifies the performance of the 4D-printed structure based on the Root Mean Square Error (RMSE) between the predicted and target coordinates. The RMSE serves as a metric to assess how well the material allocation and stimuli distribution align with the desired deformation, providing a numerical measure of the individual's effectiveness. The goal of this GA is to evolve a population of candidate solutions (individuals) towards an optimal solution that minimizes the Root Mean Square (RMS) error between the predicted and target coordinates in 4D printing as shown in Equation 1:

$$\min_{\text{epoch}\uparrow} \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[(x_i - x_i')^2 + (y_i - y_i')^2\right]} \tag{1}$$

where n is the number of columns in the part needed to be optimized, x_i and y_i are the horizontal and vertical coordinates along the central line of the deformed part, and x_i' and y_i' are the target horizontal and vertical coordinates of the central line we want to achieve.

Following the evaluation, the population is sorted based on the performance measured by the fitness function. The top 10% of individuals, deemed as elite, are selected to form a group of superior performers. These elite individuals possess favorable characteristics in terms of material allocation and stimuli distribution that contribute to achieving the desired deformation.

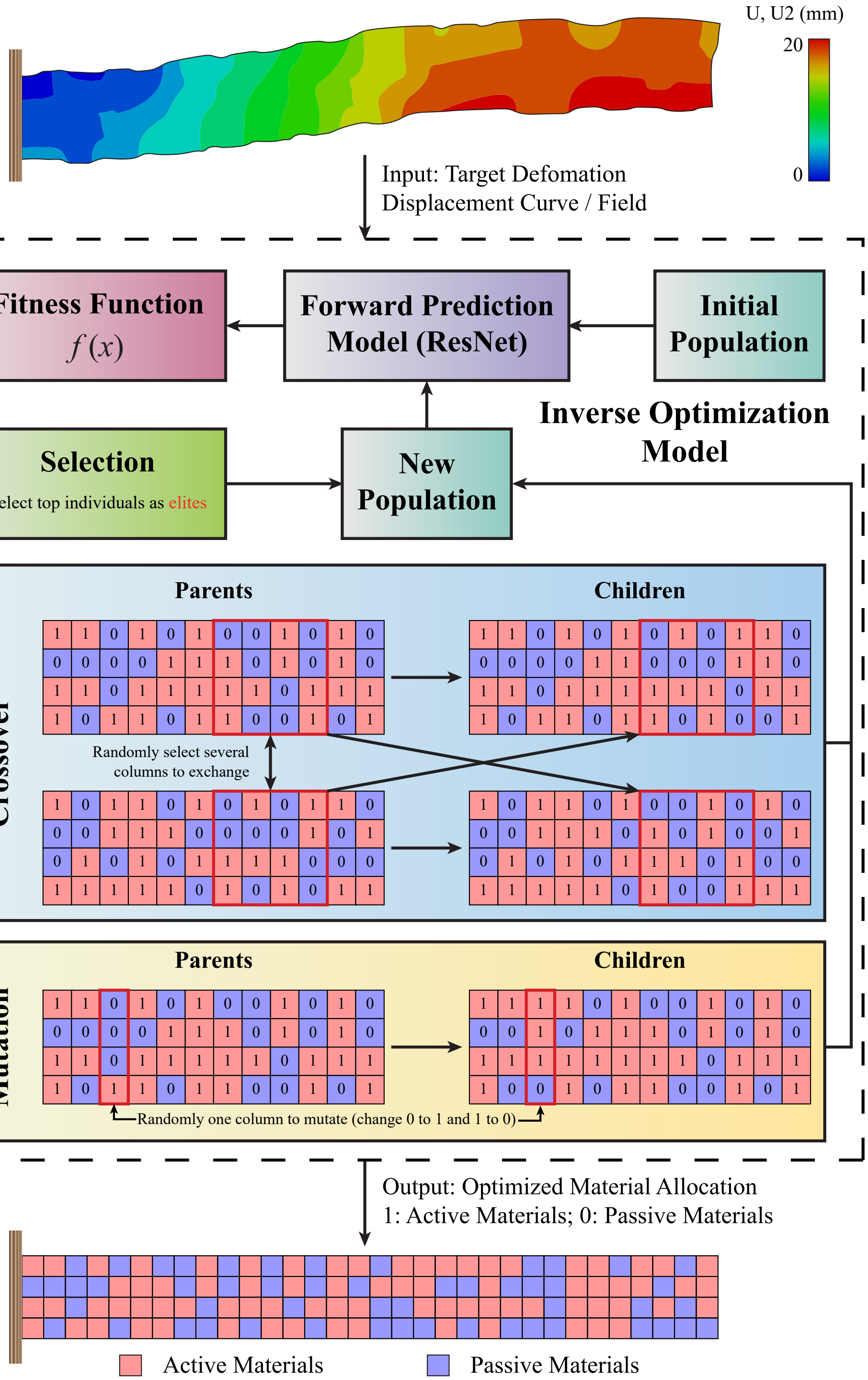

Figure 4. Inverse optimization model constructed by GA to optimize material allocation based on the predefined deformation.

The next phase involves utilizing the remaining 70% of the population for crossover operations and allocating the remaining 20% for mutation. Through crossover, genetic material from two parents (individuals) is combined to create two offspring (children), introducing diversity and potential improvements into the population. In this implementation, a two-point crossover is employed. Two random crossover columns, a and b, are selected as demonstrated in Figure 4, and the genetic materials between these columns, which are circled in red in Figure 4, are exchanged between the parents, creating two children. This process introduces diversity into the population and allows the exploration of different combinations of genetic material.

Concurrently, the mutation operation introduces random changes to the genetic material of individual members within the population. The mutation operation introduces random changes to the genetic material of an individual. A random column in the binary chromosome is selected, and the corresponding bit is flipped (from 0 to 1 or vice versa), which is illustrated in Figure 4. This operation adds randomness to the population and helps in exploring the solution space.

The combination of elite individuals and the offspring generated through crossover and mutation forms the new population for the subsequent generation. This new population, representing the second generation, undergoes evaluation once again through the fitness function. The cycle iterates, with each generation contributing to the refinement and evolution of the population toward optimal or near-optimal solutions for the 4D printing design optimization. This iterative process continues until a satisfactory level of convergence or desired performance is achieved. The genetic algorithm's ability to select and propagate the best-performing individuals, introduce variability through crossover and mutation, and iteratively refine the population underscores its effectiveness in searching for optimal solutions in the complex design space of 4D printing. In the next section (Section 5), we will validate the performance of the genetic algorithm we designed by examining the results of two case studies.

5. RESULTS

In this section, we present two case studies to evaluate the performance of the genetic algorithm designed for inverse optimization in 4D printing. The case studies involve shaping parts into a parabola and a sinusoid. The mathematical expressions for these shapes are defined as follows:

$$y = -\frac{30}{140^2}(x+80)^2 \tag{2}$$

for the parabola and

$$y = 15\cos\left[\frac{2\pi}{140}(x+80)\right] - 15 \tag{3}$$

for the sinusoid. The results of the case studies are depicted in Figure 5, where subfigures 5(a), (b), and (c) correspond to the parabola case, and subfigures 5(d), (e), and (f) correspond to the sinusoid case.

Subfigures 5(a) and (d) display the optimized results obtained from the genetic algorithm alongside the simulation results of the parts with the optimized material allocation. These results showcase a favorable alignment between the behavior of the 4D-printed part and the target deformation, demonstrating the efficacy of the optimized material allocation. To quantitatively assess the performance of genetic algorithms, subfigures 5(b) and (e) present the fitness progression for the best individual in each generation and the comparison between the target deformation and simulated deformation of the best individual after 100 generations. For the parabola shape, the root-mean-square error (fitness) approaches approximately 0.6 mm, while for the sinusoid shape, a similar level of accuracy is achieved, with the root-mean-square error near 1 mm. These errors are notably small compared to the entire length of the parts (160 mm), underscoring the robust performance of the ResNet for forward prediction and the GA for inverse optimization. Finally, subfigures 5(c) and (f) showcase the experimental results of the optimized material allocation in physical prototypes. In these cases, SMP serves as the active material, and TPU as the passive material, validating the optimized and simulated results. The parts were fabricated using an extrusion-based 3D printer with two nozzles, and the experimental outcomes align well with the optimized and simulation results.

These case studies demonstrate the effectiveness of the genetic algorithm in achieving optimized material allocations for different shapes, validating its potential for broader applications in 4D printing. The results

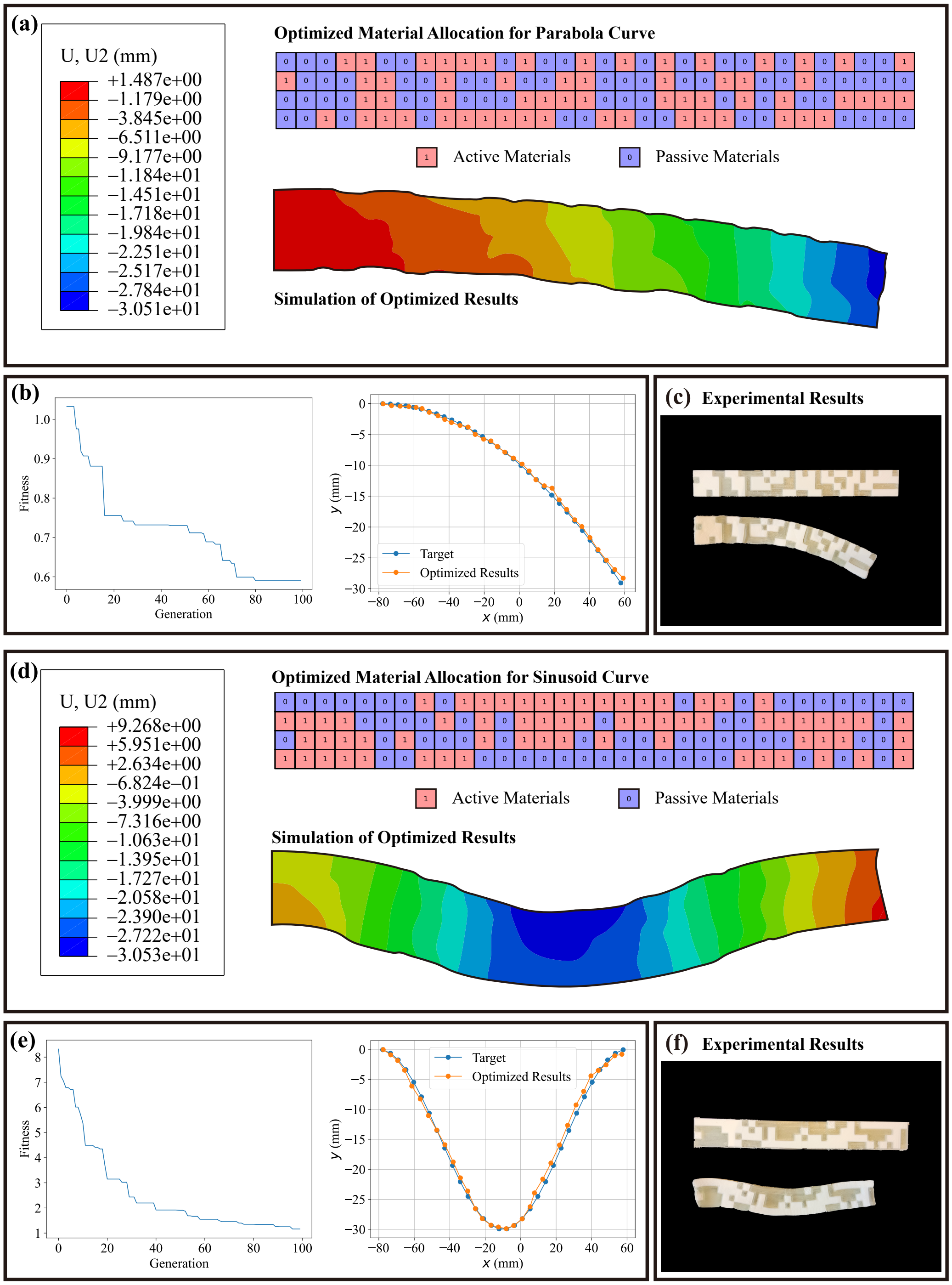

Figure 5. The results for the forward prediction and inverse optimization of two case studies. (a)(b)(c) are for parabola case. (d)(e)(f) are for sinusoid case. (a)(d). Optimized results obtained from the genetic algorithm and the simulation results of the parts with the optimized material allocation. (b)(e). The fitness for the best individual in each generation and the comparison between the target deformation and simulated deformation. (c)(f). The experimental results of the optimized material allocation.

highlight the algorithm's capability to converge towards optimal or near-optimal solutions, as evidenced by the alignment between the optimized, simulated, and experimental outcomes.

6. CONCLUSIONS AND FUTURE WORKS

In conclusion, this research paper introduces a novel approach to 4D printing design optimization, emphasizing the distribution of stimuli and materials. Leveraging the synergies of Residual Neural Network and Genetic Algorithms, our methodology provides a systematic and efficient means of orchestrating 4D printed structures to achieve specific configurations under precise stimuli and material distributions. The conventional forward design methodology in 4D printing often relies on iterative, empirical processes, leading to resource-intensive and time-consuming design optimization. Our research introduces an innovative inverse design methodology that integrates ResNet and GA, addressing both the forward prediction and inverse optimization problems. ResNet efficiently predicts the performance of 4D-printed parts based on the given design, while GA optimizes the material allocation to achieve desired configurations. The forward prediction model, constructed using ResNet, demonstrates remarkable accuracy in predicting the deformation of 4D-printed parts. The inverse optimization model, powered by GA, exhibits strong convergence towards optimal solutions. Case studies involving parabola and sinusoid shapes validate the efficacy of our methodology, with root-mean-square errors reaching as low as 0.6 mm for the parabola and approximately 1 mm for the sinusoid. The experimental results, obtained through extrusion-based 3D printing, validate the optimized material allocations. The physical prototypes align closely with the simulation and optimized results, showcasing the real-world applicability and reliability of our approach.

Future research in the domain of 4D printing design optimization offers exciting prospects, with two significant avenues for exploration identified. First, there is a need to extend the current optimization methodology to accommodate irregular shapes. While existing research has predominantly focused on rectangular or planar geometries, real-world applications often involve irregular and complex forms. The challenge lies in adapting the methodology to handle increased degrees of freedom and intricate modeling associated with irregular shapes. Future efforts should involve the refinement of machine learning models capable of handling more complex geometries and exploring techniques such as mesh-free simulations or adaptive grid structures to effectively optimize material allocation and stimuli distribution for irregular shapes. This adaptation would broaden the applicability of 4D printing in various fields, allowing for more customized and intricate designs suitable for applications such as biomedical devices, aerospace components, and architectural structures.

Second, the current optimization methodology needs to evolve to encompass 4D printing of 3D parts. The predominant focus of 4D printing has been on achieving shape changes in 2D planes, but numerous applications demand the ability to print 3D parts that undergo transformations over time. The challenge in this context is the increased complexity due to the need to consider volumetric changes and intricate internal structures. Future research should involve enhancing the methodology to accommodate the optimization of 4D printing for 3D parts, incorporating models that can predict volumetric changes, and developing optimization algorithms capable of handling three-dimensional spatial configurations. This extension of the methodology would open up new possibilities in fields such as robotics, personalized medical devices, and dynamic architectural components, enabling optimization not only for surface deformations but also for internal structures and material compositions in a volumetric context.

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