Machine learning accelerated topology optimization of nonlinear structures

Diab W. Abueidda\textsuperscript{a,b,c}, Seid Koric\textsuperscript{a,c}, Nahil A. Sobh\textsuperscript{b,d,*}

\textsuperscript{a} Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign
\textsuperscript{b} Beckman Institute of Science and Technology, University of Illinois at Urbana-Champaign
\textsuperscript{c} National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign
\textsuperscript{d} Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign

Abstract

The field of optimal design of linear elastic structures has seen many exciting successes that resulted in new architected materials and designs. With the availability of cloud computing, including high-performance computing, machine learning, and simulation, searching for optimal nonlinear structures is now within reach. In this study, we develop two convolutional neural network models to predict optimized designs for a given set of boundary conditions, loads, and volume constraints. The first convolutional neural network model is for the case of materials with a linear elastic response while the second developed model is for hyperelastic response where material and geometric nonlinearities are involved. For the nonlinear elastic case, the neo-Hookean model is utilized. For this purpose, we generate datasets, composed of the optimized designs paired with the corresponding boundary conditions, loads, and constraints, using a topology optimization framework to train and validate both models. The developed models are capable of accurately predicting the optimized designs without requiring an iterative scheme and with negligible

\* Corresponding author: Nahil Sobh

E-mail address: sobh@illinois.edu
computational time. The suggested pipeline can be generalized to other nonlinear mechanics scenarios and design domains.

**Keywords**: Nonlinear topology optimization; High-performance computing (HPC); Machine learning; Deep learning; Finite element analysis

1. Introduction

The pursuit of materials with enhanced properties yet lightweight has been of high scientific and technological interest [1-3]. Generally, such materials can be obtained by selecting the constituents a) materials, b) volume fractions, and c) architectures. The former two approaches have been studied extensively and are almost mature [4]. On the other hand, designing the architectures of materials is still an active area of research, as it allows for obtaining unprecedented properties [5-9]. The increased interest in architectured materials is related to their enhanced properties such as permeability, thermal and electrical conductivities, electromagnetic shielding effectiveness, stiffness-to-weight ratio, etc. [10, 11]. Recent advances in additive manufacturing have permitted the fabrication of such materials with complex geometries [12-14]. Attaining architectures resulting in materials with enhanced properties is usually based on intuitions, experiments, and/or bioinspiration [15, 16].

Topology optimization offers a systematic platform for obtaining new designs of materials and structural systems with optimal responses [17-23]. In topology optimization problems, one aims at identifying the optimal material distribution yielding the desired properties such as maximization of energy absorption and minimization of compliance, while still, the design constraints are satisfied. James et al. [24] developed a framework for optimizing structures where they accounted for material damage. The failure is mitigated by enforcing a constraint on the
maximum local damage intensity. Also, Russ et al. [25] used the phase field method for the fracture to increase the structural fracture resistance and strength. Geometrically nonlinear structures have also been studied, as shown in [26, 27].

Another intriguing problem in the field of topology optimization is problems involving many load cases. Zhang et al. [28] proposed a computationally-efficient randomized approach for deterministic topology optimization with many load cases. Lately, manufacturing-oriented topology optimization has experienced an increasing interest by both industry and academia, especially with recent advances in the field of additive manufacturing [29]. Also, increasing attention is observed for developing topology optimization algorithms for multi-material structures. For example, Alberdi et al. [30] developed a bi-material topology optimization framework, where hyperelastic and viscoplastic phases are combined, for maximizing energy dissipation. Additionally, Conlan-Smith et al. [31] applied topology optimization to design compliant mechanisms using functionally graded materials.

Generally, topology optimization problems are very computationally expensive due to a large number of design variables and the need for many optimization iterations before obtaining the optimal one [32]. Also, gradient-based topology optimization algorithms may suffer from the dependency on the starting point given that multiple local optima exist. In such a scenario, it is probable that the attained optimal solution is not the global optimum. These drawbacks urge many researchers to develop more efficient frameworks to determine the optimal solution. For instance, Lee et al. [33] proposed a new meta-heuristic optimization algorithm suitable for engineering applications.

Advances in high-performance computer (HPC) hardware and scalable solver algorithms have revolutionized various science and engineering fields in the last two decades allowing high fidelity
nonlinear finite element simulations of highly heterogeneous materials [34] as well as multiphysics even on the petascale computing architecture [35, 36]. The field of machine learning is no exception, and particularly deep learning has benefited from these technological advances, especially on graphics processing units (GPU). ML has been successful and effective in spam detection, image and speech recognition, discoveries of diseases and drugs, remote sensing image analysis for traffic applications, and search engines [37-39].

The use of ML algorithms has intriguingly been extended to the prediction and optimization of different materials and structural systems [40-48]. Abueidda et al. [49] developed a convolutional neural network (CNN) model that is capable of quantitatively predicting the stiffness, strength, and toughness of a two-dimensional (2D) checkerboard composite. Also, they integrated the CNN model with a genetic algorithm to perform a single- and multiple-objective (property) optimization. Furthermore, ML has shown robust performance in predicting solidification defects [50]. Also, Wei et al. [51] successfully predicted the effective thermal conductivities of composites using different ML methods. Additionally, deep learning was utilized to develop a data-driven multiphysics model for electrosurgical application [52].

Recently, deep learning has been implemented to perform optimization procedures directly without the need to involve an optimizer as in the work of Abueidda et al. [49] and Sasaki et al. [53]. This is accomplished by training the deep learning algorithms to produce images of the optimized designs given a set of boundary conditions and loads [54]. For instance, Yu et al. [55] proposed a deep learning model that is capable of identifying optimal designs without using an iterative scheme. The model was trained on synthetic data generated by an open-source code for linear elastic optimization. Moreover, Rawad and Shen [56, 57] employed a generative adversarial network, which consists of a discriminator and a generator, to optimize two-dimensional (2D) and
three-dimensional (3D) linear elastic structures. Also, Zhang et al. [58] developed a CNN model, composed of an encoder and decoder, that identifies the optimal designs in negligible time. The material they considered is a linear elastic one assuming infinitesimal strain theory. White et al. [59] developed a multiscale topology optimization framework for elastic structures using neural network surrogate model.

So far, the implementation of machine learning algorithms in topology optimization has been limited to design space with linear elastic materials undergoing small deformation. Several studies have shown that geometric and material nonlinearities significantly influence the solution of the optimization, provided that the loads are large enough to onset system nonlinearities [60-62]. In this paper, we develop two CNN models that predict the material distribution possessing the optimal response, where the first model assumes linear elastic material and small deformations, and the second model accounts for large deformations. The CNN model accounting for large deformations is developed for materials obeying the hyperelastic neo-Hookean constitutive model.

In this paper, we develop a machine learning (ML) model that performs a real-time topology optimization of materials under small and large deformation. The remainder of the paper is organized as follows: Section 2 provides an overview of the general topology optimization problem we are interested in. Section 3 scrutinizes the sample space and associated training and testing datasets. Section 4 discusses the architectures of the CNN models and their corresponding hyperparameters. Section 5 states the loss function and metrics employed in evaluating the performance of the CNN models. In Section 6, we present the results along with analysis and discussion. We conclude this study in Section 7 by summarizing the significant outcomes and discussing potential directions for future work.

2. Topology optimization
Generally, topology optimization algorithms attempt to identify the optimal material distribution within a given design space that minimizes or maximizes single or multiple objective function(s) while a set of constraints are satisfied. Topology optimization problems are solved by directly optimizing the location of the material boundary inside a design space [63], or they are solved by determining elements to be contained within a material region [24]. In this study, the latter approach is used along with the solid isotropic material penalization (SIMP) method [64]. In this study, the penalization factor is set to 3. Following this approach, each finite element (in a finite element idealization of a structure) has a density attribute $\rho_e \in [0,1]$, and each element density is considered as a design variable in the optimization problem.

Figure 1: Illustration of boundary conditions and impact of load amplitudes on the final optimized design. Optimal designs have a volume constraint of 0.35.
In the SIMP method, penalization factor $n$ is used to steer the densities $\rho$ to a value of zero or one. The parametrization is achieved by writing the total elastic energy $SE$ as

$$SE = \sum_{e=1}^{n_{ele}} \rho_e^n \int_{\Omega_e} \psi d\Omega_e$$

(1)

where $\psi$ is the strain energy density function, $n_{ele}$ denotes the total number of elements, and $\Omega_e$ is the reference configuration of element $e$ [65]. Here, we consider two types of strain energy density functions: 1) a linear elastic strain energy density function $\psi^{LE}$ and 2) a hyperelastic strain energy density function based on neo-Hookean material $\psi^{NH}$, where materials are assumed to be isotropic. The linear elastic strain energy density function is written as

$$\psi^{LE} = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl}$$

$$C_{ijkl} = \kappa \delta_{ij} \delta_{kl} + \mu \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right)$$

(2)

where $\varepsilon_{ij}$ denotes a component of an infinitesimal strain tensor, $C_{ijkl}$ is a component of the fourth-order elasticity tensor, $\delta_{ij}$ is the Kronecker delta, $u_i$ denotes a displacement component, and $(\cdot, j)$ is the gradient operator. The material parameters $\kappa$ and $\mu$ represent the bulk and shear moduli, respectively. On the other hand, the neo-Hookean strain density function [66] is expressed as

$$\psi^{NH} = C_{10} (\tilde{T}_1 - 3) + \frac{1}{D_1} (J - 1)^2$$

$$\tilde{T}_1 = \tilde{\lambda}_1 + \tilde{\lambda}_2 + \tilde{\lambda}_3$$

$$J = \det(F)$$

(3)
where $C_{10}$ and $D_1$ are material parameters, $F$ is the deformation gradient, $\bar{I}_1$ denotes the first deviatoric strain invariant, and $\bar{\lambda}_i$ are the deviatoric stretches defined as $\bar{\lambda}_i = J^{-1/3} \lambda_i$ where $\lambda_i$ are the principal stretches. In the case of small deformation, $C_{10}$ and $D_1$ reduce to $C_{10} = \frac{\mu}{2}$ and $D_1 = \frac{2}{\kappa}$.

In this paper, the objective function $G$ is defined as the compliance, sum of all elemental strain energies. $G$ is minimized over a domain composed of a structure that is subject to prescribed boundary and loading conditions as well as volume constraint $V_f$. Mathematically, this optimization problem [67, 68] can be expressed as

$$\min_{\rho} \ G(\rho) = P^T U^f + R^T U^p$$

subject to: $\frac{V(\rho)}{V_o} \leq V_f$  \hspace{1cm} (4)

where $P$ denotes the applied load vector, $R$ is the reaction force vector, and $U^f$ and $U^p$ denote the unknown free and known prescribed displacement vectors, respectively. Also, $V$ is the volume of the design structure, and $V_o$ denotes the volume of the design space. Here, we use optimization software package [68, 69] callable from a general-purpose implicit FEA code [66] to perform the topology optimization tasks at hand.

As mentioned earlier, material and geometric nonlinearities impact the optimal design especially when applied loads are sufficiently large to trigger structural and/or materials nonlinearities [60-62]. The influence of nonlinearities, on the final optimal design, is exemplified below. Consider a 2D design space consisting of 2500 (50×50) elements, where the problem stated
in equation (4) is solved with a volume constraint $V_f = 0.35$. The load and boundary conditions are as shown in Figure 1. The dimensions of the design space are $1m \times 1m$. In the case of large deformation and neo-Hookean model, the material parameters used are $C_{10} = 1$MPa and $D_1 = 1 \times 10^{-8}$ Pa$^{-1}$ (such material constants are representative of rubber mechanical properties [70]), while in the case of small deformations and linear elasticity, the materials parameters are $\mu = 2C_{10} = 2$MPa and $\kappa = \frac{2}{D_1} = 200$MPa. Figure 1 depicts the optimal designs for the elastic material with small deformations and neo-Hookean material with large deformations. The optimal design for linear elastic material with small deformation is independent of load amplitude, provided the direction is fixed. At small loads, the optimized designs obtained using the neo-Hookean hyperelasticity are identical/similar to the one attained from the linear elastic structures undergoing small deformations. However, changes in the optimized design take place when the load magnitude is increased when the neo-Hookean model is considered.

3. Data description, generation and processing

Here, two CNN models are developed, one for a linear elastic material and another for a neo-Hookean rubber-like material. A dataset is generated for each of these two material models. Each dataset is composed of many pairs of optimized designs and their corresponding boundary conditions, loads, and volume constraints. In this study, the proposed framework is illustrated using a single concentrated force (at a node on the right-hand side of the design space) while fixed displacements are imposed (at all nodes located at the left-hand side of the design space). The material properties used to generate the datasets are the same as the ones mentioned in Section 2.
Figure 2: Demonstration of the different channels.

For the sake of comparison with the work of Yu et al. [55], a $32 \times 32$ finite element mesh is used to discretize the linear elastic structure. The position, angle of incidence and the volume fraction are from a uniform random distribution with the following ranges: 1) the location of the applied force, the node selected from the set of the nodes at the right-hand side of the design space 2) the angle of the applied force ranges $\theta \in [0, 2\pi]$, and 3) the volume constraint ranges $V_f \in [0.2, 0.8]$. For each data point in the dataset, the three parameters are randomly selected using uniform distribution functions available in the open-source package Python, and then these
parameters are fed to the topology optimization framework to find the corresponding optimal
designs. Subsequently, the optimal designs are saved to a text file, including all required the
information (input and output). A total of 15,000 data pairs were generated using the NCSA’s
iForge HPC cluster with Intel/Skylake nodes each with 40 cores and 192 GB of RAM. High
throughput computing is applied to generate as many as ten data points simultaneously with the
average rate of data generation of 0.31 minutes/data point. On a personal computer with CORE i5
vPro, a single optimization task takes roughly 25 minutes to be generated. The size of the dataset
is determined by the performance of the model. The convergence condition for settling the size of
the generated dataset is to achieve a dice similarity coefficient (DSC) higher than 0.95. The
interpretation of the DSC is discussed in more details in the next section.

The next step is to arrange the generated data into a form suitable for the CNN model. With
the current selection of design space and number of elements (32 × 32), we have 33 × 33 nodes.
Each the input of each data point can be viewed as five channels (images): 1) $u_x$ with a dimension
of 33 × 33, 2) $u_y$ with a dimension of 33 × 33, 3) $P_x$ with a dimension of 33 × 33, 4) $P_y$ with a
dimension of 33 × 33, and 5) $V_f$ with a dimension of 32 × 32. $u_x$ and $u_y$ matrices have zero
components everywhere except at the nodes at the left-hand side, where fixed boundary conditions
are imposed, a value of 1 is assigned. $P_x$ and $P_y$ matrices have zero values everywhere except at
the node having the load $P$ applied. As discussed in the previous section, the magnitude of the
load, when linear elastic material with small deformation is considered, does not affect the optimal
design. Hence, $P_x$ and $P_y$ are computed as $P_x = \cos \theta$ and $P_y = \sin \theta$. Regarding the fifth channel,
we adopt a different approach to include the information about the desired volume constraint than
the approach Yu et al. [55] had used. In our approach, we use a separate channel with uniform
value of $V_f$ as part of the input, while Yu et al. [55] is passing the volume constraint information
to the latent variable as a scalar input. On the other hand, the output of each data is composed of one channel, where the values of the different pixels (elements) are the densities obtained from the optimization framework. Having said that, the pixels of all input and output channels have values ranging between zero and one. Figure 2 portrays an example of a data point; Figure 2 shows the different channels. The CNN model adopted here and discussed in the next section requires all the channels to have the same size and the number of pixels at each side of the image to be divisible by 8. This issue can be resolved by padding, adding zeros as a frame to the actual images. Given the current size of the problem, padding is done, so all the channels (inputs and outputs) possess a size of \(64 \times 64\) pixels.

For the neo-Hookean model, the considered design space has a dimension of \(1m \times 1m\), where the design space has been meshed with \(50 \times 50\) elements. Four parameters have been varied: 1) the location of the applied force, which node at the right-hand side of the design space has the load applied, 2) the magnitude of the load applied \(P \in [0, P_{\text{max}} = 150,000 \text{ N}]\), 3) the angle of the applied force \(\theta \in [0, 2\pi]\), and 4) the volume constraint \(V_f \in [0.2, 0.8]\). Like the linear elastic case, the varied parameters are randomly selected using uniform distribution. The convergence condition for determining the size of the dataset is to achieve a DSC higher than 0.95. Eighteen thousand data points had been generated to train and test the developed CNN model. In the case of hyperelasticity and large deformation, the average rate for data generation is 3.2 minutes/data point, having ten optimization tasks being solved simultaneously. Solving a single optimization task on a personal computer with CORE i5 vPro takes around 90 minutes to be completed. Figure 3 shows the data generation rates for the linear and nonlinear problems.
The next step is to arrange the generated data into a form suitable for the CNN model. The procedure is very similar to the case of the linear elastic case. The design space has $50 \times 50$ elements and $51 \times 51$ nodes. The five channels are: 1) $u_x$ with a dimension of $51 \times 51$, 2) $u_y$ with a dimension of $51 \times 51$, 3) $P_x$ with a dimension of $51 \times 51$, 4) $P_y$ with a dimension of $51 \times 51$, and 5) $V_f$ with a dimension of $50 \times 50$. $u_x$ and $u_y$ matrices are initialized with zero value, and then values of 1 are assigned at the nodes at the left-hand side, where fixed boundary conditions are imposed. $P_x$ and $P_y$ matrices are initialized with zero values, and then nonzero values are assigned at the node having the load $P$ applied. The values of the pixels corresponding to the node having the load $P$ applied are $P_x = P \frac{\cos \theta}{P_{max}}$ and $P_y = P \frac{\sin \theta}{P_{max}}$. A uniform value of $V_f$ is assigned for the volume fraction channel. The output of each data is composed of one channel, where the pixels have values equal to the densities obtained from the optimization framework. To resolve the issue of compatibility emerged from using the adopted CNN model, padding is done, so all the channels (inputs and outputs) have a size of $64 \times 64$ pixels. For both the case of the linear elastic case and neo-Hookean case, the images can be cropped to remove the padding and retrieve the original size of each problem.

![Figure 3: Data generation rates for the linear and nonlinear case.](image-url)
Figure 4: Illustration of the a) building block used in U-net, b) building used in ResUnet, and c) architecture of the ResUnet.

4. ResUnet
4.1. Architecture

The primary objective of this paper is to develop a deep CNN model to solve topology optimization problems with geometric and material nonlinearities. The adopted CNN model is based on the ResUnet proposed by Zhang et al. [39]. The ResUnet is a semantic segmentation convolutional neural network combining the privileges of the U-net and residual learning. U-net was initially proposed by Ronneberger et al. [71] to improve the performance of U-net further. U-net concatenates feature maps from different levels with the purpose of improving the segmentation accuracy. In other words, U-net combines low-level detail information and high-level semantic information to enhance segmentation accuracy. This concatenation of feature maps from different levels is not utilized in the CNN model developed by Yu et al. [55].

Generally, deeper neural networks can help get models with better performance [72]. However, very deep neural networks encounter problems such as vanishing gradients. He et al. [73] presented a deep residual learning framework to facilitate the training of very deep networks. The primary difference between the employed ResUnet [39] and conventional U-net [71] is the use of residual units instead of plain neural units as building blocks for the developed network. Figure 4a and Figure 4b portray the building blocks used in the U-net and ResUnet, respectively. A residual unit is a combination of batch normalizations (BN), rectified linear units (ReLU), and convolutional layers (Conv).

Figure 4c depicts the architecture of the ResUnet. The ResUnet is composed of three components: 1) encoder, encodes input images into compact representation, 2) decoder, retrieves the encoded representations to a pixel-wise categorization (semantic segmentation), and 3) bridge, connects the encoder and decoder. The skip connections between the encoder and decoder and within the residual units ease information propagations in forward and backward directions and
reduce the number of parameters needed. The reader is referred to the seminal paper by Zhang et al. [39] for a more in-depth discussion about the network. It is worth highlighting that we have added one residual block to the encoder and its corresponding to the decoder, as the original ResUnet architecture suggested in the seminal paper is not deep enough to predict the optimal designs for the nonlinear case, and it is sufficient for the elastic case. To have a unified framework, we used the same number of residual blocks for the linear and nonlinear cases, although the linear case does not require any modification to the original architecture.

4.2. Loss function and model evaluation

We developed two ResUnet networks, one for the small-deformation linear elastic case and one for the neo-Hookean material with nonlinearities. The models were developed and tested using Keras [74]. Also, we utilize mini-batching to increase the convergence rate and assist the CNN models to escape from local minima [75]. The same hyperparameters are used for both cases: the batch size of 64, the number of epochs of 150, and the learning rate of 0.001. We use Adam optimizer [76], which is a gradient-based stochastic optimization algorithm to train the models. The goal of the optimization problem is to find the weights $W$ of the network that minimize the loss between the ground-truth segmentation $s_i$ given input images $I_i$ and the segmentations generated by the network $Net(I_i;W)$. Here, we use the mean square error as our loss function

$$MSE = \frac{1}{n} \sum_{i=1}^{n} \|Net(I_i;W) - s_i\|^2 \quad (5)$$

where $n$ is the number of training examples. Throughout the training process, another metric is monitored in addition to the history of the MSE loss. The dice similarity coefficient (DSC) [77] is computed to evaluate the performance of the model and check its convergence. The DSC measures
the similarity between two images \([y, \bar{y}]\), where \(y\) is the ground-truth image, and \(\bar{y}\) is the predicted one, and it can be expressed as

\[
DSC = \frac{2|y \cap \bar{y}|}{|y| + |\bar{y}|}.
\]  

(6)

If two images are identical, the coefficient is equal to 1.0, while in the case of no common pixels between two images, the DSC is equal to 0.0.

Figure 5: Flowchart showing the different steps used to develop a CNN-based optimizer.

5. Results and discussion

Figure 5 presents a flowchart showing the different stages of the model development. The training of a CNN model is achieved by solving an optimization problem aiming at finding the parameters of the CNN model, so the loss function MSE is minimized. Both the CNN models
developed for the linear elastic case with small deformation and the neo-Hookean model are trained using 150 epochs. The data generated for both cases are split into training (81%), validation (9%), and testing (10%) datasets. The training dataset is the dataset used to solve the optimization problem and find the parameters of the CNN model. The validation dataset is a set of data not used to find the optimal parameters of the CNN model, but they are used to evaluate the convergence progress of the model. After each epoch, the losses obtained from the validation and training datasets are compared.

The training is done on a GPU node of iForge using a single NVIDIA v100 GPU card equipped with 32 GB of device memory. The training process takes 1.25 hrs and 1.5 hrs for the linear and nonlinear cases, respectively. Also, for comparison purposes, we run the linear case on a CPU-only iForge node with Skylake cores; the training requires 12.5 hrs, thus making an order of magnitude performance improvement on the GPU hardware. Figure 6 visualizes the training time required for the linear case when CPU-only and GPU nodes are used. Since the v100 GPU architecture has 4 GPU cards, a further performance acceleration is possible with the multi-GPU programming models, particularly with larger training data sizes, making GPU a much better choice in machine learning training.

![Figure 6](image.png)

**Figure 6:** Demonstration of training time for the linear case when CPU-only iForge node with Skylake cores and a single GPU are used.
Figure 7: The convergence history of the loss function for the CNN model developed for the case of (a) linear elasticity with small deformation and (b) geometric and material nonlinearities.

Figure 7 demonstrates the convergence history of the loss function MSE for the cases of linear elasticity with small deformation and case of geometric and material nonlinearities. For both cases, the difference between the validation and training losses is small, and this indicates that overfitting is within an acceptable level. Also, the mean DSC’s for the validation and training datasets are computed at the end of each epoch to evaluate the model. Figure 8 shows the convergence history of the DSC. After the completion of the training process, the testing dataset, which is different
from the validation dataset and not seen by the model at all through the training dataset, is used to provide a final evaluation for the developed model. The evaluation is done using the testing dataset, and it is done quantitatively by computing the mean DSC and qualitatively by randomly picking optimal designs from the testing dataset to compare between the ground-truth designs and predicted ones.

Figure 8: The convergence history of the DSC for the CNN model developed for the case of (a) linear elasticity with small deformation and (b) geometric and material nonlinearities.
Conceptually, the resulted elemental densities range from 0 to 1. Here, a threshold value of 0.5 is used to retrieve the binary nature of the solution. After the training process is accomplished, densities with values larger than 0.5 are set to 1, while densities with values smaller than 0.5 are set to 0. Let’s start with discussing the performance of the model developed for the linear elastic case with small deformation. The mean DSC is calculated using the testing dataset; the mean \( DSC = 0.958 \). This indicates that the ground-truth and predicted designs are almost identical, implying that the network is robust.

\[
\begin{array}{c|c|c|c}
\theta & V_f & \text{Ground-truth} & \text{Prediction} \\
\hline
215^\circ & 76.1\% & & \\
111^\circ & 44.3\% & & \\
127^\circ & 36.3\% & & \\
227^\circ & 27.8\% & & \\
126^\circ & 62.9\% & & \\
\end{array}
\]

Figure 9: Comparison between optimal designs for the case of linear elasticity with small deformation.
Figure 10: Comparison between optimal designs for the case of nonlinear elasticity with finite deformation.
For the sake of qualitative evaluation of the model, we pick random ground-truth designs and their corresponding predicted ones and compare them. Figure 9 shows some examples of ground-truth and predicted designs. The results obtained from the developed CNN model are almost identical to the ground-truth results. Also, in the work of Yu et al. [55], the model used provided some structural disconnections in some cases, while such disconnections did not appear in the ground-truth data. This implies that there is a kind of discrepancy in the developed model. In the present paper, the same number of elements (32 × 32) has been considered, and the issue of structural disconnections is not encountered, although fewer data points (15,000 data points compared to 100,000 data points) are used to train our model. Similar structural disconnections are also observed in the work of Zhang et al. [58]. Although the architecture of the ResUnet is more complex than those of conventional CNN models used for topology optimization problems, this complexity results in more accurate model trained on a relatively small dataset. One factor that leads to such a robust performance of the developed model is the combination of low-level information and high-level information. Figure 4 shows this information transfer from the encoder to the decoder. In addition to the architecture of the ResUnet, the random generation of data might also have led to the robust performance of the model.

Next, we show the results obtained from the model developed for the nonlinear case, neo-Hookean material with finite deformation. Figures 7b and 8b show the convergence history of the loss function and DSC, respectively. It can be implied from these figures that no major overfitting is occurring. One method to avoid overfitting is early stopping [78-80], a form of regularization. Here, we early stop the training process at 150 epochs. After the training process is completed, the ground-truth and prediction images in the testing dataset are compared; the mean DSC for the
testing dataset is 0.964. Figure 10 portrays a few examples of ground-truth and predicted designs. The results obtained from the developed CNN model almost coincide with the ground-truth results.

Also, the proposed framework can be generalized to arbitrary design spaces by adding an extra input channel defining the geometry of design spaces, prescribed displacements at different locations, and/or multiple loads (or even uniform load) leading to a multipurpose machine learning model for topology optimization. The proposed framework can be applied to other material nonlinearities such as plasticity and viscoplasticity with or without geometric nonlinearities. Additionally, one can use generative adversarial networks to refine the resolution [55]. The ability to generalize to scenarios discussed above requires data accounting for the different cases. Otherwise, such data-driven topology optimization models would lack the ability to generalize for scenarios are not accounted for during the training process. There were a few attempts to generalize such models by using different input channels, as discussed in the work of Zhang et al. [58].

Another way to use data-driven topology optimization models is to use them as initial guesses for conventional gradient-based topology optimization frameworks, as this might significantly enhance the convergence. After the training of the machine learning model is complete on HPC, the trained learnable parameters (weights and biases) can be transferred to any low-end computing platform with Keras such as a laptop, and the optimal solutions are found there instantly for any variation of input parameters. As the higher-end hardware becomes more available and affordable while the machine learning methods further mature and their confluence becomes more widely accepted by the computational mechanics communities, we believe that data-driven models will pave the way for remarkably efficient design and modeling with topology optimization and other computationally intensive numerical methods.
6. Conclusions and future work

In this paper, we develop two CNN model to predict the optimal designs in the case of linear elasticity with small deformation and the case of nonlinear hyperelasticity (neo-Hookean material) with geometric nonlinearity. The developed machine learning models are robust, and they are in a very good agreement with the designs obtained from the mathematically rigorous topology optimization frameworks, which require an expensive computational cost. We show that it is possible to generate, machine train, test, and predict data on HPC, and then produce instantly good quality nonlinear topology optimization results on a low-end computing platform such as laptops. In future work, we will work on strengthening the generalization ability of the developed data-driven topology optimization model.

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Data Availability

Data are available upon request.

References

[1] A.M. Abou-Ali, O. Al-Ketan, R. Rowshan, R. Abu Al-Rub, Mechanical response of 3D printed bending-dominated ligament-based triply periodic cellular polymeric solids, Journal of Materials Engineering and Performance, 28 (2019) 2316-2326.
[2] L.J. Gibson, M.F. Ashby, Cellular Solids: Structure and Properties, Cambridge university press1999.
[3] M.F. Ashby, H. Shercif, D. Cebon, Materials: Engineering, Science, Processing and Design, Butterworth-Heinemann2018.
[4] L. Valdevit, J. Bauer, Fabrication of 3D micro-architected/nano-architected materials, Three-Dimensional Microfabrication Using Two-photon Polymerization, Elsevier2016, pp. 345-373.
[5] W. Elmadih, W.P. Syam, I. Maskery, D. Chronopoulos, R. Leach, Multidimensional phononic bandgaps in three-dimensional lattices for additive manufacturing, Materials, 12 (2019) 1878.
[6] D.W. Abueidda, I. Jasiuk, N.A. Sobh, Acoustic band gaps and elastic stiffness of PMMA cellular solids based on triply periodic minimal surfaces, Materials & Design, 145 (2018) 20-27.
[7] D.W. Abueidda, M. Elhebeary, C.-S.A. Shiang, S. Pang, R.K.A. Al-Rub, I.M. Jasiuk, Mechanical properties of 3D printed polymeric Gyroid cellular structures: Experimental and finite element study, Materials & Design, 165 (2019) 107597.
[8] K.A. Khan, R.K. Abu Al-Rub, Viscoelastic properties of architected foams based on the Schoen IWP triply periodic minimal surface, Mechanics of Advanced Materials and Structures, (2018) 1-14.
[9] Y. Brechet, J.D. Embury, Architectured materials: Expanding materials space, Scripta Materialia, 68 (2013) 1-3.
[10] E.H.C. Castillo, N. Thomas, O. Al-Ketan, R. Rowshan, R.K. Abu Al-Rub, L.D. Nghiem, S. Vigneswaran, H.A. Arafat, G. Naidu, 3D printed spacers for organic fouling mitigation in membrane distillation, Journal of Membrane Science, 581 (2019) 331-343.
[11] D.W. Abueidda, P. Karimi, J.-M. Jin, N.A. Sobh, I.M. Jasiuk, M. Ostoja-Starzewski, Shielding effectiveness and bandgaps of interpenetrating phase composites based on the Schwarz Primitive surface, Journal of Applied Physics, 124 (2018) 175102.
[12] I. Jasiuk, D.W. Abueidda, C. Kozuch, S. Pang, F.Y. Su, J. McKittrick, An overview on additive manufacturing of polymers, JOM, 70 (2018) 275-283.
[13] W.E. Frazier, Metal additive manufacturing: A review, Journal of Materials Engineering and Performance, 23 (2014) 1917-1928.
[14] T.A. Schaedler, W.B. Carter, Architectured cellular materials, Annual Review of Materials Research, 46 (2016) 187-210.
[15] R.M. Christensen, Mechanics of cellular and other low-density materials, International Journal of Solids and Structures, 37 (2000) 93-104.
[16] J. Gao, H. Li, L. Gao, M. Xiao, Topological shape optimization of 3D micro-structured materials using energy-based homogenization method, Advances in Engineering Software, 116 (2018) 89-102.
[17] M. Bendøse, O. Sigmund, Topology Optimization: Theory, Methods and Applications, Springer, 2003.
[18] M.P. Bendsøe, N. Kikuchi, Generating optimal topologies in structural design using a homogenization method, Computer Methods in Applied Mechanics and Engineering, 71 (1988) 197-224.
[19] H. Hofmeyer, M. Schevenels, S. Boonstra, The generation of hierarchic structures via robust 3D topology optimisation, Advanced Engineering Informatics, 33 (2017) 440-455.
[20] L. Li, G. Zhang, K. Khandelwal, Design of energy dissipating elastoplastic structures under cyclic loads using topology optimization, Structural and Multidisciplinary Optimization, 56 (2017) 391-412.
[21] N. Ivarssson, M. Wallin, D. Tortorelli, Topology optimization of finite strain viscoplastic systems under transient loads, International Journal for Numerical Methods in Engineering, 114 (2018) 1351-1367.
[22] C. Le, J. Norato, T. Bruns, C. Ha, D. Tortorelli, Stress-based topology optimization for continua, Structural and Multidisciplinary Optimization, 41 (2010) 605-620.
[23] P. Michaleris, D.A. Tortorelli, C.A. Vidal, Tangent operators and design sensitivity formulations for transient non-linear coupled problems with applications to elastoplasticity, International Journal for Numerical Methods in Engineering, 37 (1994) 2471-2499.
[24] K.A. James, H. Waisman, Failure mitigation in optimal topology design using a coupled nonlinear continuum damage model, Computer Methods in Applied Mechanics and Engineering, 268 (2014) 614-631.
[25] J.B. Russ, H. Waisman, Topology optimization for brittle fracture resistance, Computer Methods in Applied Mechanics and Engineering, 347 (2019) 238-263.
[26] Q. Chen, X. Zhang, B. Zhu, A 213-line topology optimization code for geometrically nonlinear structures, Structural and Multidisciplinary Optimization, 59 (2019) 1863-1879.
[27] K. Matsui, K. Terada, S. Nishiwaki, Topology optimization with CAMD for structures undergoing finite deformation, IUTAM Symposium on Topological Design Optimization of Structures, Machines and Materials, Springer, 2006, pp. 333-342.
[28] X.S. Zhang, E. de Sturler, G.H. Paulino, Stochastic sampling for deterministic structural topology optimization with many load cases: Density-based and ground structure approaches, Computer Methods in Applied Mechanics and Engineering, 325 (2017) 463-487.
[29] J. Liu, A.T. Gaynor, S. Chen, Z. Kang, K. Suresh, A. Takezawa, L. Li, J. Kato, J. Tang, C.C. Wang, Current and future trends in topology optimization for additive manufacturing, Structural and Multidisciplinary Optimization, 57 (2018) 2457-2483.
[30] R. Alberdi, K. Khandelwal, Bi-material topology optimization for energy dissipation with inertia and material rate effects under finite deformations, Finite Elements in Analysis and Design, 164 (2019) 18-41.
[31] C. Conlan-Smith, A. Bhattacharyya, K.A. James, Optimal design of compliant mechanisms using functionally graded materials, Structural and Multidisciplinary Optimization, 57 (2018) 197-212.
[32] S. Watts, W. Arrighi, J. Kudo, D.A. Tortorelli, D.A. White, Simple, accurate surrogate models of the elastic response of three-dimensional open truss micro-architectures with applications to multiscale topology design, Structural and Multidisciplinary Optimization, (2019).
[33] K.S. Lee, Z.W. Geem, A new meta-heuristic algorithm for continuous engineering optimization: harmony search theory and practice, Computer Methods in Applied Mechanics and Engineering, 194 (2005) 3902-3933.
[34] J. Li, A. Saharan, S. Koric, M. Ostoja-Starzewski, Elastic–plastic transition in three-dimensional random materials: massively parallel simulations, fractal morphogenesis and scaling functions, Philosophical Magazine, 92 (2012) 2733-2758.
[35] M. Vázquez, G. Houzeaux, S. Koric, A. Artigues, J. Aguado-Sierra, R. Arfís, D. Mira, H. Calmet, F. Cucchietti, H. Owen, Alya: Multiphysics engineering simulation toward exascale, Journal of Computational Science, 14 (2016) 15-27.
[36] S. Koric, A. Gupta, Sparse matrix factorization in the implicit finite element method on petascale architecture, Computer Methods in Applied Mechanics and Engineering, 302 (2016) 281-292.
[37] J.H. Witten, E. Frank, M.A. Hall, C.J. Pal, Data Mining: Practical Machine Learning Tools and Techniques, Morgan Kaufmann2016.
[38] S. Lafon, A.B. Lee, Diffusion maps and coarse-graining: A unified framework for dimensionality reduction, graph partitioning, and data set parameterization, IEEE Transactions on Pattern Analysis and Machine Intelligence, 28 (2006) 1393-1403.
[39] Z. Zhang, Q. Liu, Y. Wang, Road extraction by deep residual U-net, arXiv preprint arXiv:1711.10684, (2017).
[40] A. Agrawal, A. Choudhary, Perspective: Materials informatics and big data: Realization of the “fourth paradigm” of science in materials science, Apl Materials, 4 (2016) 053208.
[41] G.X. Gu, C.-T. Chen, D.J. Richmond, M.J. Buehler, Bioinspired hierarchical composite design using machine learning: simulation, additive manufacturing, and experiment, Materials Horizons, 5 (2018) 939-945.
[42] C. Bisagni, L. Lanzi, Post-buckling optimisation of composite stiffened panels using neural networks, Composite Structures, 58 (2002) 237-247.
[43] S. Banga, H. Gehani, S. Bhilare, S. Patel, L. Kara, 3D topology optimization using convolutional neural networks, arXiv preprint arXiv:1808.07440, (2018).
[44] K.M. Hamdia, H. Ghasemi, X. Zhuang, N. Alajlan, T. Rabczuk, Computational machine Learning representation for the flexoelectricity effect in truncated pyramid structures, Computers, Materials & Continua, 59 (2019) 79-87.
[45] K.M. Hamdia, H. Ghasemi, Y. Bazi, H. AlHichri, N. Alajlan, T. Rabczuk, A novel deep learning based method for the computational material design of flexoelectric nanostructures with topology optimization, Finite Elements in Analysis and Design, 165 (2019) 21-30.
[46] H. Hofmeyer, J.M. Davila Delgado, Coevolutionary and genetic algorithm based building spatial and structural design, Artificial Intelligence for Engineering Design, Analysis and Manufacturing, 29 (2015) 351-370.
[47] M. Papadrakakis, N.D. Lagaros, Y. Tsompanakis, Structural optimization using evolution strategies and neural networks, Computer Methods in Applied Mechanics and Engineering, 156 (1998) 309-333.
[48] C.-Y. Lin, S.-H. Lin, Artificial neural network based hole image interpretation techniques for integrated topology and shape optimization, Computer Methods in Applied Mechanics and Engineering, 194 (2005) 3817-3837.
[49] D.W. Abueidda, M. Almasri, R. Ammourah, U. Ravaiolli, I.M. Jasiuk, N.A. Sobh, Prediction and optimization of mechanical properties of composites using convolutional neural networks, Composite Structures, 227 (2019) 111264.
[50] S. Feng, H. Zhou, H. Dong, Using deep neural network with small dataset to predict material defects, Materials & Design, 162 (2019) 300-310.
[51] H. Wei, S. Zhao, Q. Rong, H. Bao, Predicting the effective thermal conductivities of composite materials and porous media by machine learning methods, International Journal of Heat and Mass Transfer, 127 (2018) 908-916.
[52] Z. Han, Rahul, S. De, A deep learning-based hybrid approach for the solution of multiphysics problems in electrosurgery, Computer Methods in Applied Mechanics and Engineering, 357 (2019) 112603.
[53] H. Sasaki, H. Igarashi, Topology Optimization Accelerated by Deep Learning, IEEE Transactions on Magnetics, 55 (2019) 1-5.
[54] X. Lei, C. Liu, Z. Du, W. Zhang, X. Guo, Machine learning-driven real-time topology optimization under moving morphable component-based framework, Journal of Applied Mechanics, 86 (2019) 011004.
[55] Y. Yu, T. Hur, J. Jung, I.G. Jang, Deep learning for determining a near-optimal topological design without any iteration, Structural and Multidisciplinary Optimization, 59 (2019) 787-799.
[56] S. Rawat, M.H.H. Shen, Application of adversarial networks for 3D structural topology optimization, SAE International 2019-01-0829, 2019.
[57] S. Rawat, M.-H.H. Shen, A novel topology optimization approach using conditional deep learning, arXiv preprint arXiv:1901.04859, (2019).
[58] Y. Zhang, A. Chen, B. Peng, X. Zhou, D. Wang, A deep convolutional neural network for topology optimization with strong generalization ability, arXiv preprint arXiv:1901.07761, (2019).
[59] D.A. White, W.J. Arrighi, J. Kudo, S.E. Watts, Multiscale topology optimization using neural network surrogate models, Computer Methods in Applied Mechanics and Engineering, 346 (2019) 1118-1135.
[60] M. Osanov, J.K. Guest, Topology optimization for architected materials design, Annual Review of Materials Research, 46 (2016) 211-233.
[61] K. Maute, S. Schwarz, E. Ramm, Adaptive topology optimization of elastoplastic structures, Structural Optimization, 15 (1998) 81-91.
[62] T. Buhl, C.B. Pedersen, O. Sigmund, Stiffness design of geometrically nonlinear structures using topology optimization, Structural and Multidisciplinary Optimization, 19 (2000) 93-104.
[63] G. Allaire, F. Jouve, A.-M. Toader, Structural optimization using sensitivity analysis and a level-set method, Journal of Computational Physics, 194 (2004) 363-393.
[64] M.P. Bendsoe, Optimal shape design as a material distribution problem, Structural Optimization, 1 (1989) 193-202.
[65] A. Klarbring, N. Strömberg, Topology optimization of hyperelastic bodies including non-zero prescribed displacements, Structural and Multidisciplinary Optimization, 47 (2013) 37-48.
[66] ABAQUS, ABAQUS Documentation, Dassault Systèmes, 2014.
[67] T.E. Bruns, D.A. Tortorelli, Topology optimization of non-linear elastic structures and compliant mechanisms, Computer Methods in Applied Mechanics and Engineering, 190 (2001) 3443-3459.
[68] FE-DESIGN GmbH, SIMULIA Tosca Structure Documentation 8.1, SIMULIA, 2014.
[69] W. Saleem, M.A. Khan, S.R. Ch, Formulation and execution of structural topology optimization for practical design solutions, Journal of Optimization Theory and Applications, 152 (2012) 517-536.
[70] J.J. Wang, J. Lee, C.S. Woo, B.K. Kim, S.B. Lee, An experimental study and finite element analysis of weatherstrip, International Journal of Precision Engineering and Manufacturing, 12 (2011) 97-104.
[71] O. Ronneberger, P. Fischer, T. Brox, U-net: Convolutional networks for biomedical image segmentation, International Conference on Medical image computing and computer-assisted intervention, Springer, 2015, pp. 234-241.
[72] C. Szegedy, W. Liu, Y. Jia, P. Sermanet, S. Reed, D. Anguelov, D. Erhan, V. Vanhoucke, A. Rabinovich, Going deeper with convolutions, Proceedings of the IEEE conference on computer vision and pattern recognition, 2015, pp. 1-9.

[73] K. He, X. Zhang, S. Ren, J. Sun, Deep residual learning for image recognition, Proceedings of the IEEE conference on computer vision and pattern recognition, 2016, pp. 770-778.

[74] F. Chollet, Keras, GitHub, https://github.com/fchollet/keras, 2015.

[75] G.E. Hinton, A practical guide to training restricted Boltzmann machines, Neural networks: Tricks of the trade, Springer2012, pp. 599-619.

[76] D.P. Kingma, J. Ba, Adam: A method for stochastic optimization, arXiv preprint arXiv:1412.6980, (2014).

[77] K.H. Zou, S.K. Warfield, A. Bharatha, C.M. Tempany, M.R. Kaus, S.J. Haker, W.M. Wells III, F.A. Jolesz, R. Kikinis, Statistical validation of image segmentation quality based on a spatial overlap index1: scientific reports, Academic Radiology, 11 (2004) 178-189.

[78] C.M. Bishop, Pattern Recognition and Machine Learning, springer2006.

[79] C. Zhang, S. Bengio, M. Hardt, B. Recht, O. Vinyals, Understanding deep learning requires rethinking generalization, arXiv preprint arXiv:1611.03530, (2016).

[80] I. Goodfellow, Y. Bengio, A. Courville, Deep learning, MIT press2016.