Composite Design Optimization via DeepONet

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Abstract: Composite and porous materials have been widely applied in various industries including aerospace, civil infrastructure, automobile, bioengineering, electronics, etc., where the microstructural and topological design for tailored properties has been of importance. In this work, we hope to construct a novel topology optimization approach for composite structures based on the recent development of operator regression. Inspired by the recent work on applying machine learning algorithms for materials design, we aim to train surrogate models based on deep operator networks and obtain the top candidates, i.e. digital representation of the materials and structures, for desired properties, e.g., high stiffness, low stress-concentration, etc.

Objective and Goals

In this project, the main objective and focus are to **design novel composite structures via trained surrogate models from operator regression**. The key idea here is to search for the "good design" via on-the-fly inference from surrogate models. Since many researchers in the field have already applied many ML surrogate models for inverse design, we here are essentially curious about the performance of DeepONet on inverse design applications. We are curious about how those models behave as surrogates for inverse design. Based on such, we identify three main goals:

- Generate a reasonable amount of training sets[2] with finite element methods (FEM).
- Successfully implement and train the surrogate model via DeepONet.
- Search for "good design" via inferences from DeepONet (or other potential models) in the properties' library for the optimal design.

Ideally, we can obtain the optimal structures of targeted composites from a reasonable amount (a lot less than a grid or random search) of simulations. For the application scenarios, we hope to start with a simple composite design process using FEM as a general demonstration. If time allows, I hope to implement my own research, designing three-dimensional biocomposites (or biofilm-based porous materials) using the proposed DeepONet approaches.

Our Proposed Approach

We use DeepONet to create the surrogate model for design optimization. The general design scheme is shown in Figure 1. The design process begins with the training sets: we (plan) to first generate 50 sets using FEM simulations; the data are then to be trained via DeepONet as illustrated in Figure 3 (Supplementary). The trained DeepONet is then to be used to infer and create the "properties' library". The top candidates of excellent performance on the desired properties are then to be selected and used for further (high fidelity) FEM verification. Once the simulations' results meet the desired criteria, such structures are then filtered and selected as optimal designs to guide real-world industrial applications.

Mathematical Modeling

The simulation used in our training data is finite element simulations of linear elastic mechanics problems, which basically gives the relation between stress and strains:

$$\sigma = \mathbf{C}\epsilon$$

where $\sigma = \sigma_{ij}$ and $\epsilon = \epsilon_{ij}$ are stresses and strains, respectively, are 2×2 matrices for our simplified two-dimensional cases. The stiffness matrix $\mathbf{C}$ maps from ϵ to σ via the linear elastic constitutive relations[3]:

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[2]that is, not "too much" yet still enough to train surrogate models.

[3]can be also extended to other constitutive models

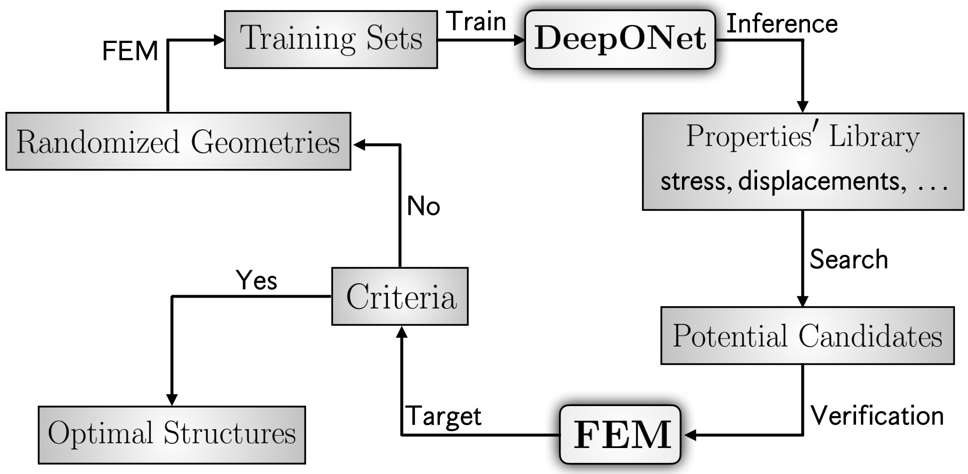

FIGURE 1. The schematic illustration of the DeepONet-based design scheme.

$\mathbf{C} \in \mathbb{R}^{2\times2\times2\times2} : \mathbb{R}^{2\times2} \to \mathbb{R}^{2\times2}$. The displacements and strains (kinematics) follows: $\epsilon = \nabla\mathbf{u}$. Boundary conditions can be expressed in the form $\Omega(\partial, \sigma, \epsilon) = 0$. Substitute the balance laws one can solve for the targeted mechanics problems. Due to the limitation of the page, I won't go into too much detail about the basics here.

The other important math model is operator regression. As simplified as I can, Karniadakis and coworkers extended the work by Chen & Chen[4] to a mapping of input and output continuous function spaces and regressor learn the labels mapped on the output space:

$$G(u)(y) \approx \sum_{k=i}^{p} \underbrace{b_k(u(x_1), u(x_2), ..., u(x_m))}_{\text{branch net}} \underbrace{a_k(y)}_{\text{trunk net}}$$

where u and y are input and output function spaces, and x_i are the input continuous functions (digitalized by sensors in the form of discretized data points). Details can be found in Ref. [5][5].

PROBLEM FORMULATION

To apply this scheme for design deployment, we propose a 5×5 discretized space to generate pores in selected units. The selection of the pore units is the optimization process. A basic materials base is shown in Figure 2: a discretized basis consisting of the pore units, where we select a specific amount, e.g., 10, of them to set as fiber (or hard materials), and the rest are recognized as a matrix (soft materials). The constitutive model for the two materials is all linear elastic. We may expect a specific pore distribution to end up with a lower stress concentration.

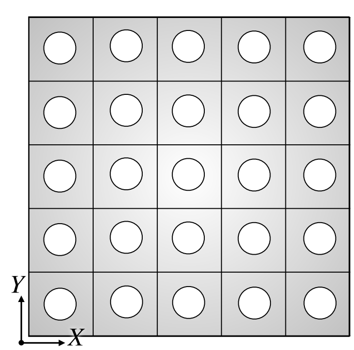

FIGURE 2. The schematic for basic design formulation.

[4]DOI: 10.1109/72.286886

[5]Due to the page limit, many mathematical details are neglected in the proposal

Supplementary to Main Proposal

Statement of Significance

Obtaining decent designs of materials, structures, and systems, via probing the design variables is a long-standing problem in various scientific and engineering fields. Traditional topology optimization methods search for the "good design" via computing the gradient for the design space optimum is problem-flexible yet contains two main drawbacks: (1) the design is easy to be trapped in the local minimum and sensitive to the initial point(s)[6]; (2) takes more computational burden since has to do the gradient iterations for different initial schemes[7]. Recently, with the rapid developments of machine learning (ML) and its applications in optimization and computing, many researchers have applied various ML frameworks for different design problems, such as CNN for porous graphene design [11], Gaussian process for antibiofilm nanosurfaces design [14], CNN for composites design [3]. Despite the plural of exciting works, we here apply DeepONet for such an inverse design process considering three major novelties: (1) The theoretical foundation of operator regression is well established, traced back to the 90s. Related analyses are easy to be carried out. (2) The mapping using deep networks is based on labeling of the FEM meshing, which is much more computationally efficient compared with the widely used CNN methods. (3) The design process from our proposed DeepONet allows the user to directly input the design variables as a vector, which is theoretically sensible and easier to interpret. TO elaborate on this point in detail, the design of branch-trunk nets structures allows mapping from different continuous functional spaces, in simple words, one can input different matrices of different dimensions for operator regression. We borrow this convenience and design the branch net to take the design variables directly as input.

Background and Review

Machine Learning as Surrogate Models for Mechanics Problems. There have been rapid developments in applying ML for mechanics problems, mainly on how to construct *surrogate models* efficiently. From the multiscale perspective, *ab initio* based machine learning potential bridges the scale from quantum (or more rigorously in the scale of density functional theory) to the molecular regime [1, 16]. There are follow-up works adopting the same ideology bridging the molecular scale to the mesoscale, i.e. the coarse-grained regime [17] by E and coworkers. Up to micro and macro scale, there are many works that leverage high-resolution simulations and use various ML tools to build up surrogate models, like predicting bubble dynamics [15]. In general, the key idea is to train a surrogate model using the regressor of convenience with the corresponding optimization algorithms, i.e. GD, SGD.

Scientific Machine Learning Integrates Domain Knowledge for Accurate Inferences. There is a rise in the efforts to integrate known theories in ML since around 2015. Some representative works include using sparse regression to identify dynamics systems' mathematical expression, and encoding dynamical systems by Brunton and coworkers [2, 10, 7]; encoding known equations into neural networks via automatic differentiation by Karniadakis and coworkers [8, 9, 13]; and most importantly and recently, applying universal approximation theory to map functional spaces and extended to deep nets called operator regression [5]. There are some major debates on the performances and structures of different operator networks, more specifically debates over deep operator networks and Fourier neural operator [6, 4]. Despite the plural network architectures, we here are interested in how DeepONet performs on actual materials design and deployment applications.

Machine Learning for Design Optimization: Wide Applications. Since the huge success of ML and their various works on surrogate modeling as mentioned in the previous paragraphs, scholars of the materials, structures, and mechanics communities may start to wonder: how to release the real power of ML into more practical applications of a better use for mechanics? To me, design optimization is one of the answers. Many researchers like to apply CNN[8] to create a "picture-to-picture mapping" problem and further use this surrogate for design applications such as the design of desalination graphene [12], low thermal conductivity graphene [11], composite structures [3], etc. However, the convolutional layer

[6] also happens a lot in gradient-based optimization for other applications

[7] for SciML the training is also taxing yet the inference would be "on-the-fly" once the model is trained.

[8] thanks to its established success in facial recognition and related visual applications

in CNN introduces a much higher computational burden for storing and iterating the weights during the optimization process. We hence suggest creating direct mappings from numerical data to data through operator regression for efficiently training and inferences.[9]

Training of DeepONet

The training of the DeepONet surrogate is illustrated in detail in Figure 3: A branch net and a trunk net mapping the input of design variables and corresponding meshing, respectively, connected for operator regression for the desired output. In the proposed approach, we plan to use von Mises' stress field as the desired output for mapping. We also hope to use less stress concentration as the target to avoid stress-induced damage initiation in materials.

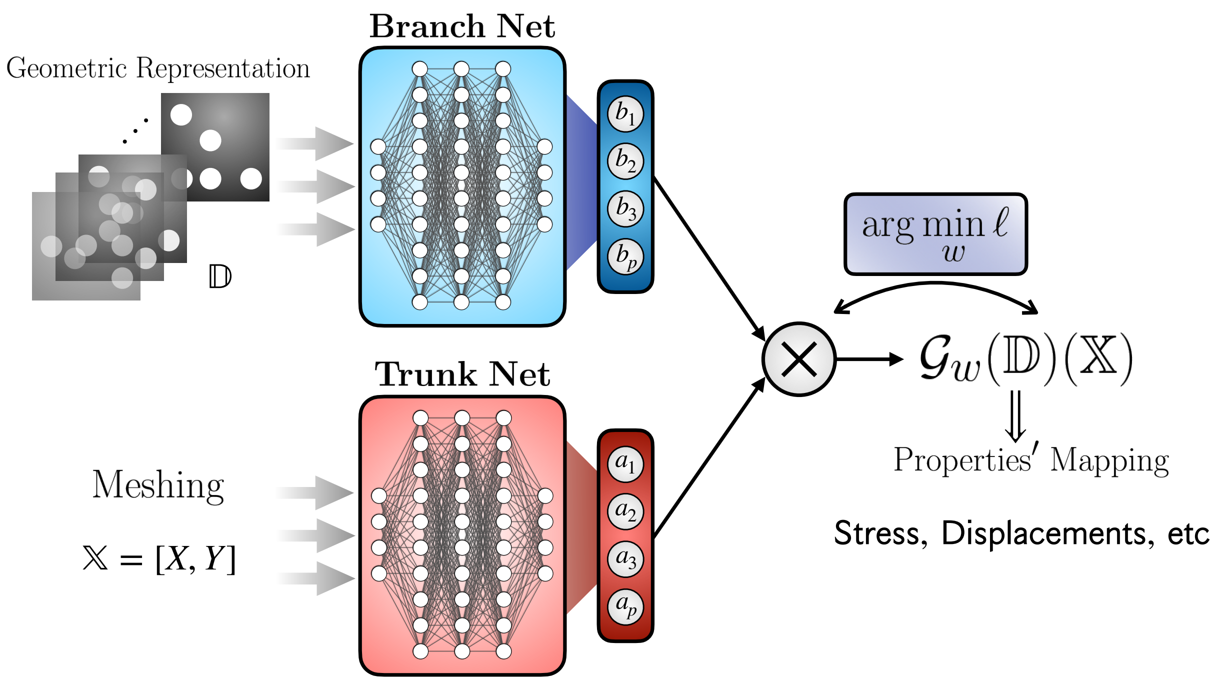

Figure 3. The detailed implementation of constructing the surrogate model of the composites' properties' calculation using DeepONet. The Branch Net takes the vectorized design parameters as input and the Trunk Net takes the generated corresponding meshing as input. The output via operator regression is the desired properties, e.g., von Mises' stress. The trained model can infer on-the-fly.

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