DH-Net: Deformed Microstructure Homogenization via 3D Convolutional Neural Networks

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Abstract

With the rapid development of additive manufacturing, microstructures are attracting both academic and industrial interests. As an efficient way of analyzing the mechanical behaviors of microstructures, the homogenization method has been well studied in the literature. However, the classic homogenization method still faces challenges. Its computational cost is high for topological optimization that requires highly repeated calculation. The computation is more expensive when the microstructure is deformed from a regular cubic, causing changes for the virtual homogeneous material properties. To conquer this problem, we introduce a fine-designed 3D convolutional neural network (CNN), named DH-Net, to predict the homogenized properties of deformed microstructures. The novelty of DH-Net is that it predicts the local displacement rather than the homogenized properties. The macroscopic strains are considered as a constant in the loss function based on minimum potential energy. Thus DH-Net is label-free and more computation efficient than existing deep learning methods with the mean square loss function. We apply the shape-material transformation that a deformed microstructure with isotropic material can be bi-transformed into a regular structure with a transformed base material, such that the input with a CNN-friendly form feeds in DH-Net. DH-Net predicts homogenized properties with hundreds of acceleration compared to the standard homogenization method and even supports online computing. Moreover, it does not require a labeled dataset.

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and thus can be much faster than current deep learning methods in training processing. DH-Net can predict both homogenized material properties and micro-mechanical properties, which is unavailable for existing DL methods. The generalization of DH-Net for different base materials and different types of microstructures is also taken into account, as demonstrated in the results.

Keywords: Homogenization theory, deformed microstructures, convolutional neural networks, deep learning, mechanical properties

1. Introduction

Microstructures are ubiquitous in natural objects and possess a variety of excellent physical properties. With the rapid development of additive manufacturing, microstructures are more and more utilized in many industrial fields like mechanical, aerospace, and civil engineering, e.g., design for lightweight and high strength [1]. Almost all materials possess heterogeneous and complex microstructures at a certain scale, contributing to superior mechanical, thermal, and electromagnetic properties. However, understanding the behavior of such microstructures is not an easy task for their distinct geometry, volume fraction, and constituents properties. It is nearly impossible to experiment on a large number of microstructural samples with different geometry and physical properties, attributed to time and cost consumption. Also, simulating the entire body leads to computationally expensive and high memory storage requirements [2].

To address these problems, homogenization theory has been developed as a multiscale technique in past decades. The homogenization method relies on the morphology of microstructures and evaluates the stress-strain relationship at the macro-scale by solving the boundary value problem associated with the micro-scale. Here the micro-scale sample refers to representative volume element (RVE) to unit-cell for regular microstructures. The boundary conditions are commonly considered with periodic displacement and anti-periodic traction. Predicting the homogenized physical properties has been considered as a basis of many applications, i.e., topological optimization [3, 4, 5, 6], and functional structural design [7, 8, 9, 10]. The most popular computational architecture is the voxel-based two-scale microstructure framework, in which the object is first partitioned into a voxel grid as a coarse scope, then the periodic microstructures are filled into the grid with pre-homogenized material properties for simulation and optimization.
Although the voxel-based two-scale microstructure framework reaches a trade-off between design accuracy and simulation efficiency, it still faces the inherent drawbacks that the clipped boundary voxels induce fragment structures and significant simulation errors. An alternative way to conquer this issue is to replace voxels with hexahedra to achieve well boundary conforming and adaptive cell size [11, 12]. However, deformed microstructures filled in hexahedral cells exhibit a different mechanical behavior compared to that in voxel grid [13]. This means that we need to take shape parameters of deformed microstructures into account for the homogenization method. Tozonoi et al. [14] introduced a rhombic microstructure family for irregular lattices in a 2D plane. They pre-homogenized a geometry-material space for a two-scale framework, in which both microstructure parameters and a shape parameter (rhombic angle $\alpha$) were used for structural design. However, this method is somewhat limited as it only suits isotropic microstructures, but most periodic microstructures are orthotropic in practice. Also, it only covers the rhombus in 2D. For more general deformation, e.g., parallel hexahedra in 3D, the geometry-to-material mapping will become a dense high dimension space with prohibitive pre-homogenizing costs.

For 3D deformed orthotropic microstructures, we introduce a 3D convolutional neural network, called DH-Net, in place of the deformed homogenization method to predict the macroscopic physical properties of deformed microstructures. We construct a novel loss function based on minimum potential energy (MPE) theory instead of mean square (MSE) loss function. It allows our dataset to be constructed without the ground truth; otherwise, pre-computing ground truth is as time-consuming as building the geometry-to-material space. There has not been any deep learning (DL) method used to predict the macroscopic properties of deformed microstructures. Most DL methods for predicting microstructure properties, i.e., convolutional neural network (CNN), require voxel-based inputs for their innately fit for DL operations, like conv and pooling. However, deformed microstructures lose this edge. So we construct a new dataset consisting of deformed microstructures and provide a shape-material transformation to convert shape parameters into the change of base materials. It can be used in both DH-Net and other current methods without changing their input as well.

DH-Net speeds up hundreds of times than numerical homogenization methods and even achieves real-time predicting. Benefiting from the prediction of displacements, DH-Net can provide more mechanical properties (e.g., strain and stress distribution, yield strength, and shear strength) than
the existing DL method, which only can predict homogenized material properties. Furthermore, our approach has better generalization performance, e.g., DH-Net performs better to predict homogenized material properties for such microstructures not involved in the dataset. We also provide a post-processing step; as a result, prediction results can vary depending on the input material parameters without retraining the network.

The main contributions of our work are as follows.

- We propose a 3D convolutional neural network based on 3D U-Net, named DH-Net, and a novel loss function based on minimum potential energy theory to predict the homogenized material properties of deformed microstructures. DH-Net is label-free, more time-efficient than current deep learning methods, and highly generalizable to arbitrary microstructures.

- We construct a dataset of deformed microstructures based on parallel hexahedra and introduce a shape-material transformation method to convert the calculation of the homogenization of deformed microstructures into that of unit cells, taking the migration of the homogenized material in the presence of different base materials into account.

- We predict the displacements for deformed microstructures and more microscope mechanical properties, e.g., strain and stress distribution, yielding strength, and shear strength, apart from homogenized material properties.

2. Related Work

2.1. Homogenization theory

Homogenized material properties are widely used for many structural design problems to replace heterogeneous composites and microstructures, as it significantly reduces the computational cost of simulation and optimization. The homogenization theory, originally developed to solve partial differential equation (PDE) problems, is to estimate the homogenized macroscopic properties from the response of its underlying microstructure, thereby allowing to substitute the heterogeneous material with an equivalent homogeneous one [2, 15].

These approaches have three main categories, including (i) Analytical methods, i.e., Voigt and Reuss assumptions [16, 17] specified the upper and
lower bound of the macroscope properties. While universal and very simple, these bounds do not carry any geometry information of the microstructures and take only the in-homogeneity volume fraction into account. They typically provide rough estimates of the overall material properties and are unreliable for complex nonlinear structures. (ii) Semi-analytical methods, e.g., Mori–Tanaka model [18, 19], the self-consistent scheme [20, 21], the generalized self-consistent scheme [22, 23], and the differential method [24, 25]. These methods are mainly based on the mean-field approximation and approximate the interaction between the phases. The extension of these models is to account for the elastic behavior of composite materials. (iii) Numerical methods have been introduced to perform various analyses over the representative volume element (RVE), such as Voronoi cell finite element [26, 27], fast Fourier transform (FFT) [28], boundary element (BE) method [29], and finite element (FE) discretization [30, 31, 32].

Although the numerical method is known to be computationally expensive, it has been more focused since it has shown to be adequate to high heterogeneous materials and microstructures, both linear and nonlinear problems. Liu et al. [33] build mechanical property profiles for microstructures using asymptotic homogenization to help users select the desired microstructure from alternatives and improve specific microstructure properties in microstructural design. Homogenization methods for deformed microstructures have been concerned recently. Tozonoi et al. [14] homogenize a rhombic microstructure family for irregular lattices in a 2D plane, whose homogenized material properties are always isotropic. Our paper follows this idea and extends to 3D orthotropic microstructures.

2.2. Data-driven homogenization approach

Many works have been recently developed to decrease the computational cost and increase the accuracy of the multiscale analysis. These methods are typically based on employing a database to map the effective behavior from macroscopic information directly. Several works [8, 9, 10, 34, 35, 36] presented to pre-build a geometry-material space by homogenization method offline, then query target homogenized material properties by interpolation method. However, these methods require a large number of samples to ensure accuracy, and each material space is only applicable to a specific type of microstructures.
Figure 1: The whole pipeline of DH-Net includes three main steps: (a) pre-processing that transforms the deformed microstructure into a regular microstructure with the transformed base material, (b) predicting microscope displacements and then homogenized material properties through a convolutional neural network, (c) post-processing that re-transforms properties for the deformed homogenized space.

With the popularity of data science, many machine learning (ML) methods have been introduced to microstructure analysis and design. Fritzen et al. [37] propose a two-stage data-driven homogenization approach for nonlinear solids. Lookman et al. [38] employ an active learning approach to navigate the search space for identifying the candidates for guiding experiments or computations. Ford et al. [39] explore the use of supervised ML to predict the mechanical properties of a family of two-phase materials using their microstructural images. However, ML techniques heavily depend on feature engineering and require expert knowledge, which is time-consuming and limited to their applications.

Recently, deep learning (DL) approaches showed significant success in a great variety of applications due to the capability to search for the most salient features to be learned automatically. Hence, many research attempts utilized DL methods, such as neural networks (NN), convolutional neural networks (CNN), and graph convolutional networks (GCN), to predict the homogenized material properties. Le et al. [40] propose a decoupled computational homogenization approach for nonlinearly elastic materials using NN to approximate the effective potential. Lu et al. [41] adopt NN to establish a surrogate model for electric conduction homogenization. Yang et al. [42] implement a deep learning feature-engineering-free approach to the prediction of the microscale elastic strain field in a given three-dimensional voxel-based microstructure of a high-contrast two-phase composite. Rao et
al. [15] propose a three-dimensional CNN to predict the effective material properties RVEs with random spherical inclusions. Vlassis et al. [43] integrate geometric deep learning and Sobolev training to generate a family of finite strain anisotropic hyperelastic models that predict the homogenized responses of polycrystals previously unseen during the training.

Although these methods showed that they could replace the homogenization method and predict homogenized properties instantly for a given microstructure, it is pretty time-consuming to construct a dataset including ground-truth labels, as ground-truth still needs to be computed by the standard homogenization method. Like the geometry-material space method, current DL methods tend to overfit specific kinds of microstructures involved in the dataset instead of showing generalization for other types of microstructures. Besides, these methods are only considered with microstructures that have cubic shapes, while deformed microstructures are not taken into account.

3. Architecture of DH-Net

As shown in Figure 1, the whole processing is divided into three main steps in this paper, including (a) the pre-processing to transform the deformed microstructure into a regular microstructure with the transformed base material, (b) a convolutional neural network to predict microscope displacements and then obtain homogenized material properties, (c) a post-processing step to re-transform properties for the deformed homogenized space. We first introduce the architecture of DH-Net in this section. The pre-processing and post-processing steps, which are based on shape-material transformation, are described in Section 4.2.

3.1. Asymptotic homogenization

DH-Net depends on a theory of numerical homogenization method called asymptotic homogenization [44, 45], including two main steps, the localization step and integration step.

In the localization step, a periodic microstructure Ω is first discretized into $N^3$ voxels. Under a periodic boundary condition, the microscope displacements $u$ are computed by

$$Ku = f,$$  \hspace{1cm} (1)
where the stiffness matrix $K$ is assembled by the stiffness matrix of each voxel $\Omega_e$. The local stiffness matrix $K_e$ is expressed by

$$K_e = \int_{\Omega_e} B^T_e C^b B_e d\Omega_e,$$

(2)

where $B_e$ is a local strain displacement matrix. Similarly, the traction $f$ are assembled by the force of each voxel resulting from given macroscope strains $\varepsilon$ with six independent strain directions,

$$f_{e_i} = \int_{\Omega_e} B^T_e C^b \varepsilon_i d\Omega_e,$$

(3)

where these six macro-strains are presented as

$$\varepsilon_1 = \{1, 0, 0, 0, 0, 0\}, \; \varepsilon_2 = \{0, 1, 0, 0, 0, 0\},$$

$$\varepsilon_3 = \{0, 0, 1, 0, 0, 0\}, \; \varepsilon_4 = \{0, 0, 0, 1, 0, 0\},$$

$$\varepsilon_5 = \{0, 0, 0, 0, 1, 0\}, \; \varepsilon_6 = \{0, 0, 0, 0, 0, 1\}.$$  

At the stage of integration, the homogenized material properties $C^H$ are integrated by the linear relationship of macroscope strains and microscope strains using a volume average operator

$$C_H = \frac{1}{|\Omega|} \sum_{e=1}^{N^3} (I - B_e u_e)^T C^b (I - B_e u_e) d\Omega_e,$$

(5)

where $I$ is a $6 \times 6$ identity tensor. Its more general and simplified form is

$$C_H = \frac{1}{|\Omega|} \sum_{e=1}^{N^3} (u_e - u_0)^T K_e (u_e - u_0) d\Omega_e,$$

(6)

where $u_0 = K_e / f_e$.

### 3.2. Loss function

Unlike the DL methods that predict homogenized properties directly, DH-Net predicts the microscope displacements $u$ from given macroscope strains $\varepsilon$ in the localization step through a 3D convolutional neural network $N(\theta)$. The main difference is that we construct a novel loss function $L$ relying on
the minimum potential energy (MPE) theory instead of the mean square loss function. Our loss function is formulated as

$$L(u) = \sum_{i=1}^{6} \frac{1}{2} u_i^T Ku_i - u_i^T f_i,$$

whose gradients $\frac{\partial L}{\partial u}$ are expressed as $\sum_{i=1}^{6} Ku_i - f_i$. This loss function is reasonable and has been commonly used in many works [e.g. 46] that solve finite element (FE) problems by ML and DL methods. Besides, we note that no matter how the input parameters change, the macroscopic strain $\varepsilon$ remains the same, so we can compute the external traction $f_e$ for each voxel directly by Eq. 3. The macroscopic strains $\varepsilon$ can be regarded as universal and implicated ground-truth in the loss function of DH-Net. That means our energy-based loss function as a criterion is enough to minimize DH-Net to convergence, unlike other loss functions that need extra ground truth. It benefits since pre-computing ground-truth in constructing the dataset by asymptotic homogenization is extremely time-consuming, just as well as building the geometry-material space for interpolation.

3.3. DH-Net structure

We construct DH-Net with a U-Net style structure, as shown in Figure 2. The input of DH-Net is a fourth-order tensor with size $N^3 \times 36$, in which the shape parameters, microstructure morphology, and its base materials are in
consideration. The output of DH-Net is $N^3 \times 18$ in size, which consists of six local displacements under the load of six macro-strains $\varepsilon$, just like those computed by numerical homogenization.

U-Net is proposed by Ronneberger et al. [47] for biomedical image segmentation. Compared with the fully connected network (FCN), it implements up-sampling operation in U-Net to replace pooling operation and adds jump connection module with more elegant network architecture. In practice, we observe that using up-sampling and down-sampling operations on microstructure space benefits the connection and the exchanges of weight parameters, so U-Net can be localized and achieve better results with only a small number of training data. Therefore, U-Net is applied for the prediction of 3D microstructure properties in our work.

As illustrated in Figure 2, DH-Net contains a contracting path (left side) and an expansive path (right side) that is symmetrically distributed at the beginning and end of the network. The contracting path contains two repeated convolution blocks, each consisting of a 3D convolutional layer and a rectified linear unit (ReLU). A batch-norm operation is performed at the end of each convolutional layer to reduce the impact of data distribution. The convolution kernel is $3 \times 3 \times 3$, and padding is set to 1. The convolution block is followed by a $2 \times 2 \times 2$ maximum pooling layer with a stride 2 for down-sampling. At each down-sampling step, we double the number of feature channels. On the expansive path, the feature map clipped from the contracting path is connected with the up-sampled results, and then the convolution operation is carried out. Different from the compression path, the number of channels is halved after each convolution. Finally, we use a $1 \times 1 \times 1$ convolution layer to map the result to a $N^3 \times 18$ tensor.

4. Dataset Generation

4.1. Selection of parameters

We consider three distinct types of parameters in dataset construction: shape, microstructure, and base material.

4.1.1. Shape parameters

To reduce the complexity of deformed microstructure homogenization, we assume all microstructures that belong to our dataset are limited to parallel hexahedra. Then, we search the optimal pairs from deformed hexahedra
Figure 3: The linear map $F$ and its inverse $G$ between cubic unit $P$ and parallel hexahedron $Q$ are considered as the transformation of coordinate basis with three scaling variables $l_x, l_y, l_z$ and three angle variables $\alpha_{xy}, \alpha_{yz}, \alpha_{xz}$, respectively.

to parallel hexahedra by geometry processing, e.g., iterative closest point algorithm [48], to minimize matching errors.

Thanks to parallelism, any deformed hexahedron $Q$ in the dataset can be derived from a cubic unit $P$, whose orthogonal coordinate system is deformed into a non-orthogonal basis by a linear transformation. As shown in Figure 3, the linear mapping $F : P \rightarrow Q$ is parameterized by 6 variables, which are the magnitude scales of coordinate axes and the angles between them. We use $l_x, l_y, l_z$ and $\alpha_{xy}, \alpha_{yz}, \alpha_{xz}$ to denote the scale variables and angle variables, respectively.

In this paper, we set scale variables $l_x, l_y, l_z \in [\frac{2}{3}, \frac{3}{2}]$ and angle variables $\alpha_{xy}, \alpha_{yz}, \alpha_{xz} \in [75^\circ, 90^\circ]$. To eliminate rotational errors, we specify that the X-axis of the deformed hexahedron is $[1, 0, 0]^T$, and the $X-Y$ plane is perpendicular to $[0, 0, 1]^T$. Therefore, we can express the mapping relationship as the product of the scaling matrix $T(l_x, l_y, l_z)$ and the shear matrix $S(\alpha_{xy}, \alpha_{yz}, \alpha_{xz})$, that is $F = ST$. Similarly, we can calculate linear mapping $G : Q \rightarrow P$ by inversing $F$ in turn.

4.1.2. Microstructure parameter and its base material

For a given microstructure $\Omega$ in the dataset, regardless of its geometric parameters, it is voxelized into a 0-1 3D tensor, whose size is $N^3$. It is divided into two parts, of which the solid part is 1. To be specific, the usage of our approach is limited to linear elasticity. Therefore, we implement isotropic material $C^b(E, v)$ as the base material in the dataset, which can be easily calculated by Young’s modulus $E$ and Poisson ratio $v$. 

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Figure 4: (a) In dataset construction, a deformed microstructure with an isotropic base material $C^b$ is converted into a normal microstructure with a transformed base material $\tilde{C}^b$ by shape-material transformation; (b) the inverse procedure after computing the homogenized material properties $\tilde{C}^H$ of the cubic unit, aims to recover the homogenized material $C^H$ on the parallel hexahedron.

However, using only the solid part as input in the 3D CNN training will result in incorrect output. That is because some weights in the neural network lack backward gradients so that they are never updated. Hence, we have to assume that the microstructure in the dataset is composed of a two-phase composite of hard and soft materials, in which the hard material property $C^{bh}$ is set to $E = 1, v = 0.3$, but the soft one $C^{bs}$ is set to $E = 10^{-6}, v = 0.3$.

4.2. Shape-material transformation

As we know, there has not been a deep learning method used to predict the macroscope properties of deformed microstructures up to now. Most DL methods for predicting microstructure properties require voxel-based inputs for their innately fit for DL operations, like conv and pooling. However, deformed microstructures lose this edge.

To address this problem, we adopt a shape-material transformation introduced by [14]. As mentioned above, shape deformation $F: P \rightarrow Q$ can be considered as a non-orthogonal basis, in which a hexahedron $Q$ is expressed
as a cubic unit. If displacements $u$ satisfy the elastic equation $K(C)u = f$ on a unit domain, $\bar{u}$ and $\bar{f}$ are the displacement and force expressed on the non-orthogonal basis, respectively, Tozonoi et al. have proved that they also satisfy the elastic equation

$$\tilde{K}(\tilde{C})\tilde{u} = \tilde{f},$$  \hfill (8)

only if the base material $C^b$ is transformed by

$$\tilde{C}^b_{ijkl} = G_{pi}G_{qj}G_{rk}G_{sl}C^b_{pqrs},$$  \hfill (9)

where $G : Q \rightarrow P$ is the inverse map from a hexahedron to a cubic unit. This can be verified directly by changing variables in Eq. 1. Also, the homogenized elastic tensor $C^H$ can be expressed in terms of $\tilde{C}^H$ by the inverse relation:

$$C^H_{ijkl} = F_{pi}F_{qj}F_{rk}F_{sl}\tilde{C}^H_{pqrs}.$$  \hfill (10)

Therefore, the whole processing of DH-Net works as follows:

1. Compute $\tilde{C}^{bh}$ and $\tilde{C}^{bs}$ by Eq. 9, then construct $\tilde{C}^{bh} \times \Omega + \tilde{C}^{bs} \times (1 - \Omega)$ as input (Figure 4a);
2. Predict microscope displacements $\tilde{u}$ using DH-Net, and calculate homogenized elastic tensor $\tilde{C}^H$;
3. Recover homogenized tensor $C^H$ on the orthogonal basis by Eq. 10 (Figure 4b).

4.3. Dataset Construction

For each input to DH-Net, we first transform base materials $\tilde{C}^{bh}$ and $\tilde{C}^{bs}$ and reshape each base material ($6 \times 6$ elastic tensor) into a vector, then combine the microstructure $\Omega$ with its base materials by $\tilde{C}^{bh} \times \Omega + \tilde{C}^{bs} \times (1 - \Omega)$, whose size is $N^3 \times 36$. We construct the dataset by sampling each shape parameter 5 times at equal intervals.

We adopt a typical microstructure, Tubular Gyroid (TG), a type of triply periodic minimal surface (TPMS) in the dataset and uniformly sample the TG structure 40 times with the volume fraction within $[2.4\%, 33\%]$. Combined with the shape parameters, the dataset is of 625K samples, which leads extraordinarily time-consuming training process. So we performed experiments on randomly pruning the dataset into 1%, 5% and 10% sets, and found that the dataset with 10% random sample points (totally 62.5K) achieved the excellent balance of convergences and prediction errors.
5. Results and Discussions

5.1. Setting of DH-Net

We evaluate the performance of the proposed DH-Net for predicting homogenized properties of deformed properties. DH-Net is built on Pytorch 1.8.1 using Python 3.9, trained on a platform equipped with NVIDIA GeForce GTX 1080Ti GPU with Intel Core i3-7980CPU@2.6GHz. We first conduct a set of hyper-parameters (e.g., batch-norm, learning rate, architecture) to modulate optimal networks. Then, the well-trained network is used to predict the displacements of deformed microstructures on the non-trained testing dataset and calculate homogenized properties for them. The performance of DH-Net is evaluated the error between predicting results and their corresponding ground-truth $C^H_g$, given by

$$\delta = \frac{|C^H - C^H_g|}{|C^H_g|}, \quad (11)$$

where $C^H_g$ is computed by a MATLAB version homogenization method [49].

We shuffle the dataset and select 80% of the sample points as the training set and the remaining 20% as the test set to validate the prediction error of DH-Net. For the training procedure, we implement Adam [50] as the optimizer of DH-Net, whose learning rate is set to $10^{-4}$ and the batch size is set to 8.

5.2. Time-consuming analysis

The training process takes 12 hours, of which 30% of the time is spent evaluating prediction errors. However, to satisfy the current DL prediction
method with MSE loss function, it needs at least 180 hours to compute ground-truth for our dataset. The dataset has 62.5K sample points in total, and the computation of each sample point needs 6s to 15s using the numerical homogenization method. As for the interpolation approaches of geometry-material space, it takes ten times as long as the construction of ground-truth since we only randomly select 10% samples in the dataset construction.

We also compare the prediction time of DH-Net with the numerical homogenization method, as shown in Figure 5. The time cost for numerical homogenization is positively correlated with the volume fraction of the microstructure. Here, for the model with volume fraction from 2% to 33%, the solving time increases from 5.83s to 14.77s. On the contrary, DH-Net gains hundreds of speed-up independent of the volume fraction, which takes 5.3ms for all volume fractions.

5.3. Convergence and error distribution

As shown in Figure 6a, the loss of DH-Net tends to converge after 30 epochs. We take one batch out of 100 batches to evaluate the prediction error during the training process, and the plot of prediction error shows a similar downward trend with loss. Both of them witness a rapid decline at first, then decrease slowly and fall into their minimal point after 30 epochs, where the average prediction error remains stable at 1%.

After the training process, the test set is used to validate the performance of trained DH-Net, and the distribution of prediction errors is plotted in
The test results are similar to the prediction error of the last epoch of the training process, where the average prediction error for the whole test set is 0.95%.

The prediction error of DH-Net has achieved the same level of SOTA results after 30 epochs and can support most applications, e.g., two-scale microstructure modeling. Increasing epochs can further reduce the prediction error, but it may be less significant than former epochs, limited by its built-in drawbacks like floating point accuracy and interpolation error.

5.4. Demonstration of prediction results

To further evaluate the performance of DH-Net, we demonstrate examples in our dataset to show more visualization results. As shown in Figure 7, we provide three deformed TPMS-TG microstructures with the same volume fraction (10%) but different shape parameters. Since Young’s modulus is a crucial variable to depict the material properties, we compared their plots of Young’s modulus $E$ with the prediction results of the numerical homogenization method and DH-Net. We observe that the predicted results of DH-Net (right) are incredibly close to those of the numerical homogenization method (middle column). The prediction error for the three examples is only 0.9%, 0.5%, 1.2%, respectively.

Apart from predicting homogenized material properties as current DL methods, DH-Net can benefit the prediction of microscope mechanical properties, i.e., local stresses, attributing to the choice of displacement as output. As shown in Figure 8, we input the predicted displacements of three deformed microstructures, then obtain their worst-case stress distribution. Theoretically, we can calculate and visualize mechanical properties of all microstructures introduced by [33], e.g., local strains and stresses, yield strength, and shear strength. These properties heavily rely on the prediction of displacements are much helpful in microstructure design but are not available with existing DL methods.

5.5. Generalization of DH-Net

The generalization of DH-Net is considered for two aspects, including types of microstructures and their base materials.

The generalization of microstructural types benefits from that the original purpose of DH-Net is to learn how to solve PDE equations, which is more universal and less possible to overfit. Although it was trained on a
Figure 7: Three deformed TPMS-TG microstructures with the same volume fraction (10%) but different shape parameters (left column). From top to bottom, their shape parameters are $(1, 1, 1, 75°, 75°, 75°)$, $(2/3, 2/3, 3/2, 90°, 90°, 90°)$, $(2/3, 2/3, 3/2, 75°, 75°, 75°)$, respectively. The second and third column are the plots of predicted Young’s modulus given by numerical homogenization (middle) and DH-Net (right).
Figure 8: The worst-case stress distribution of the three examples in Figure 7.

\[ \sigma_{\text{max}} = 146.5 \quad \sigma_{\text{max}} = 276.4 \quad \sigma_{\text{max}} = 412.2 \]

Figure 9: Left: The average prediction errors of three different type of microstructures by DH-Net and other convolutional neural network to predict elastic tensor directly. Right: Trends of loss and prediction error for three different type of microstructures using DH-Net as pre-trained network.

microstructure dataset built by TPMS-TG, it is able to predict the properties of other types of microstructures such as Kelvin, Octet-Truss, and ORC-Truss, etc. As shown in Figure 9 (left), the prediction errors of DH-Net are significantly lower than those of existing DL methods to predict elastic tensor directly, e.g., [15]. In addition, DH-Net can be used as a well pre-training network for any microstructure. We construct datasets for other types of microstructures and use DH-Net as a pre-trained network. The prediction errors for other kinds of microstructure fall back to 0.02 after 6 epochs, which is relatively faster than that without a pre-trained network (Figure 9 right).

In constructing the dataset we assume that the properties of the base
material are $E = 1, v = 0.3$ and $E = 10^{-6}, v = 0.3$. However, we may change the properties of the base materials in practice, depending on what we used. To avoid retraining network due to changes in the base material, we implement an approach called CLM Theorem based on invariant properties of the stress, by which we can easily calculate the change of homogenized material when the base material is changed. It was first introduced by [52] but is only suitable to plane elasticity and isotropic homogenized materials.

Considering that most types of microstructures are 3D and orthotropic, we use its improved approach introduced by [53], which relies on Hill’s condition and field fluctuation and is well suited for 3D and orthotropic microstructures. Supposing that the base material $C^b(E^b, v^b)$ is replaced with another base material $C^b(\hat{E}^b, \hat{v}^b)$, then the orthotropic homogenized material is changed from $C^H(E_i, v_{i,j}, G_{i,j})$ to $C^H(\hat{E}_i, \hat{v}_{i,j}, \hat{G}_{i,j})$, $i, j \in \{x, y, z\}$ by

$$
\hat{E}_i = \frac{\hat{E}^b}{E^b} E_i, \\
\hat{v}_{i,j} = v_{i,j} - (v^b - \hat{v}^b) \frac{E_i}{E^b}, \\
\frac{1}{2\hat{G}_{i,j}} = \frac{E^b}{E^b} \frac{1}{2G_{i,j}} - (v^b - \hat{v}^b).
$$

(12)

6. Conclusion

In this paper, we propose DH-Net, a U-Net style conventional neural network, to predict the homogenized material properties of deformed microstructures. Other than existing DL methods, DH-Net predicts the microscope displacements under macroscope strains and periodic boundary conditions. We construct a novel loss function based on MPE theory, with no need for ground-truth labels in dataset construction. We also construct a new dataset consisting of deformed microstructures and provide a shape-material transformation that combines shape parameters into the input.

DH-Net can speed up the prediction of homogenized material properties hundreds of times. More importantly, DH-Net is label-free, superior to existing DL methods that require highly time-consuming ground-truth dataset construction. DH-Net can evaluate many mechanical properties using displacements, e.g., worst-case stress distribution, yield strength, and shear strength, which are unavailable for other DL methods output elastic
properties directly. Besides, DH-Net takes the generalization of both microstructure types and their base materials into account. It can be used well in different based materials and different types of microstructures.

DH-Net still has improvement space. First, the shape parameters in the dataset are within $[75°, 90°]$ for angles and $[2/3, 3/2]$ for scaling. We expect to expand the range of shape parameters and introduce more types of microstructures in the future. Besides, the accuracy of DH-Net is lower than the numerical homogenization method, and its training time is still rather long. We note that the computation of loss function still has improvement space, e.g., to reduce the illness of loss function, and the first-order Adam optimizer also has improvement space. In the future, we plan to use numerical strategies, like building pre-conditioners to boost solving efficiency and implement higher-order optimizers, i.e., L-BFGS, to reduce iteration steps.

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