

Transfer learning for enhancing the homogenization-theory-based prediction of elasto-plastic response of particle/fiber-reinforced composites

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Abstract

We recently proposed the adaptive incrementally affine method as a novel homogenization scheme that enables accurate prediction of the nonlinear mechanical response of particulate-reinforced composites under cyclic or multiaxial loading conditions. However, being a mean-field homogenization method that relies on the solution of Eshelby's inclusion problem, the aforementioned method does not provide accurate predictions when the shape of the reinforcement has a high aspect ratio or the interaction among reinforcements becomes significant. Herein, we propose a combined theoretical and data-driven approach in which the homogenization method is followed by transfer learning to enhance the prediction of the nonlinear mechanical response of particle/fiber-reinforced composites. We trained a deep neural network (DNN) with a massive stress-strain curve dataset of a composite subjected to uniaxial loading in the elasto-plastic regime based on the adaptive incrementally affine homogenization method; then, we fine-tuned the pre-trained DNN via transfer learning with a relatively small dataset based on time-consuming three-dimensional (3D) finite element analyses (FEA). The transfer learning approach exhibited better predictive performance than the DNN directly trained only with the FEA dataset did, for a wide range of reinforcement volume fractions and shapes. With transfer learning, the DNN exploits the knowledge learned from the homogenization theory to perform a new learning task on a small dataset from 3D FEA. The combined theoretical and data-driven approach proposed herein can be extended to other composite analyses when experiments or simulations require excessive time and cost for a large dataset and the applicability of the homogenization theory is limited.

1. Introduction

With the addition of various forms of reinforcements, reinforced composites have evolved to outperform single-phase materials. Predictions of the effective responses of such composites are crucial for efficient machine element design and structural optimization across a variety of industries. As the first generation of composite analysis, homogenization methods based on analytical formulations have been investigated for many decades [1, 2]. These methods entail lower computational costs compared with finite element analysis (FEA) or experiments but have limitations owing to the use of mathematical assumptions. For example, the mean-field homogenization theory is valid under a relatively small volume fraction of reinforcement ($<20\%$) because the mean-field assumption is violated as the volume fraction increases [3-6]. If a homogenization method relies on the solution of Eshelby's inclusion problem, reinforcements with a non-ellipsoidal shape can only be approximately treated [7-9]. As the second generation of composite analysis, the finite element method (FEM) has been extensively employed with the advancement of computational capability [10]. However, the nonlinear behavior of materials and structural complexity significantly increase the computational cost of the FEM, which limits its applicability. Recently, as the third generation of composite analysis, data-based machine learning [11, 12], which incorporates machine learning techniques into the composite analysis [13-16], has drawn significant attention. Once a machine learning model has been trained, it can immediately predict the outputs for given input values; however, it requires a large amount of data for reliable prediction.

Each method has advantages and disadvantages, and thus, a single method would not be a satisfactory or universal route toward efficient composite analyses. For example, the homogenization theory enables exceedingly fast prediction of the effective properties of composites, but its accuracy and applicability are limited. Meanwhile, both three-dimensional

FEM analysis and direct experimental measurements offer highly accurate predictions of composite properties but at the expense of excessive time or cost. However, the accuracy and efficiency of composite analysis can be significantly improved by training a machine learning model with a large but less accurate dataset based on the homogenization method and then improving the machine learning model with an accurate but small dataset using the FEM or through experiments. Herein, we propose a combined theoretical and data-driven framework to realize such a hybrid composite analysis via transfer learning.

Various mean-field homogenization methods have been proposed based on Eshelby's solution [1]. For linear elastic composites, the Mori–Tanaka [2, 17], differential [18, 19], and double-inclusion [20] methods have been widely used. For composites exhibiting nonlinearity, such as viscosity or plasticity, the incrementally affine [21, 22], incrementally secant [23, 24], and adaptive incrementally affine [25, 26] methods have been proposed. These methods are reliable when the shape of the reinforcement is close to a sphere and the volume fraction of the reinforcement is small. However, many technologically important composites are synthesized with a variety of forms and a relatively large volume fraction of reinforcement, which limits the applicability of homogenization methods. In contrast, deep learning techniques have been employed to predict the mechanical properties of two-dimensional checkerboard composites [15, 27-29] or three-dimensional linear elastic composites [30, 31]. It is well known that with more data, the generalization of a deep neural network (DNN) model is improved for unseen data. When a sufficiently large training dataset does not exist, the performance of DNNs becomes inferior to that of conventional machine learning techniques such as linear regression, support vector machine, or decision tree-based algorithms [16]. However, it is often difficult to obtain sufficiently large datasets owing to time and cost problems.

Given that homogenization methods have limitations in terms of accuracy and that

DNNs require excessively large amounts of data, we propose incorporating transfer learning techniques to composite analysis. Transfer learning is a method that uses a model trained once for a particular task as a starting point for training a second model [32]. Therefore, transfer learning is used when it is difficult to obtain sufficient data [33-37]. The representative volume element (RVE) of a composite with reinforcements having a high aspect ratio in the nonlinear regime entails substantial computational costs associated with FEM; then, it becomes difficult to obtain the amount of data required for machine learning. In the present study, we show that a framework combining the homogenization theory and transfer learning can predict the effective behavior of the elasto-plastic composite efficiently and reliably; a sufficiently large dataset is generated using the homogenization theory for the initial DNN training, at a low computational cost; subsequently, the pre-trained DNN is fine-tuned using relatively small FEM data obtained via transfer learning. The workflow of our transfer-learning framework is illustrated in Fig. 1.

The remainder of this paper is organized as follows. The constitutive equations for modeling the elasto-plastic behavior are summarized in Section 2.1. A description of the data generation is presented in Section 2.2. The adaptive incrementally affine and yield reduction methods are briefly introduced for the homogenization data. The face-centered-cubic (FCC) structured RVE is introduced for FEM data. The procedure for applying transfer learning is described in Section 3. The results for the ellipsoidal particle-reinforced composite are presented in Section 4.1. The results for the fiber-reinforced composites are included in Section 4.2. The conclusions are presented in Section 5.

Boldface letters indicate second- or fourth-order tensors and non-bold face letters indicate scalar values; $(:)$ denotes a double contraction, as $\mathbf{a}:\mathbf{b} = a_{ij}b_{ji}$; $(\mathbf{A}:\mathbf{b})_{ij} = A_{ijkl}b_{lk}$.

2. Material modeling and numerical method

2.1. Material modeling

We consider composites containing an elasto-plastic matrix. We note that the methodology employed in this study can be applied to a variety of other composite materials as well that show viscoelastic or viscoelastic-viscoplastic responses. In the elasto-plastic constitutive model, the total strain ($\boldsymbol{\varepsilon}$) is divided into the elastic part ($\boldsymbol{\varepsilon}^e$) and plastic part ($\boldsymbol{\varepsilon}^p$):

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p. \quad (1)$$

Then, the Cauchy stress ($\boldsymbol{\sigma}(t)$) is determined as follows:

$$\boldsymbol{\sigma}(t) = \mathbf{C} : \boldsymbol{\varepsilon}^e = \mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p). \quad (2)$$

Assuming isotropic materials, the fourth-order stiffness tensor ($\mathbf{C}$) is expressed as,

$$C_{ijkl} = \frac{E\nu}{(1-2\nu)(1+\nu)} \delta_{ij}\delta_{kl} + \frac{E}{2(1+\nu)} (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \quad (3)$$

where E is Young's modulus, ν is Poisson's ratio, and δ is the Kronecker delta.

Rate-independent isotropic hardening is assumed for plasticity. The yield function (f) is defined as follows:

$$f(\sigma_{eq}, p) \equiv \sigma_{eq} - (\sigma_y + R(p)) \quad \text{where } \sigma_{eq} = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}} \quad (4)$$

$$p = \sqrt{\frac{2}{3} \boldsymbol{\varepsilon}^p : \boldsymbol{\varepsilon}^p}, \quad (5)$$

where $\mathbf{s}$ is the deviatoric part of the Cauchy stress, σ_{eq} is the von Mises stress, σ_y is the yield stress, R is the hardening stress, and p is the accumulated plastic strain. For hardening responses beyond the yield, isotropic hardening with the power law is adopted:

$$R(p) = kp^n \quad (6)$$

where k is the hardening modulus, and n is the hardening exponent. Thus, isotropic elasto-

plastic behavior can be modeled with five parameters: Young's modulus, Poisson's ratio, yield stress, hardening modulus, and hardening exponent.

2.2. Data generation with a homogenization method and 3D FEM modeling

Considering that the reinforcement is much stiffer than the matrix materials in most composites, the composite is assumed to be an elasto-plastic matrix reinforced with linear elastic particle/fiber. Its composition can be characterized by nine parameters related to the elastic properties (Young's modulus E_0 , Poisson's ratio ν_0) and plastic properties (yield stress σ_y , hardening modulus k , hardening exponent n) of the matrix, as well as the elastic properties (Young's modulus E_1 , Poisson's ratio ν_1), aspect ratio (AR), and volume fraction (f_1) of the reinforcements. After normalizing E_1 , σ_y , and k with E_0 , the input parameters can be reduced to a set of eight dimensionless parameters. With the normalized eight parameters as the input, we set the effective stress-strain curve of the composite subjected to uniaxial loading as the output. We consider a wide range of input parameters to cover a variety of elasto-plastic composite behaviors, as presented in Table 1.

The adaptive incrementally affine method with yield reduction is adopted as the homogenization method because it has been shown to offer highly accurate predictions of the complex nonlinear mechanical response of particulate-reinforced composites beyond the elastic regime, under cyclic and multiaxial loading. In the regime where the assumption of micromechanics-based mean-field homogenization theory holds, that is, a small volume fraction of a reinforcement having an ellipsoidal shape with an aspect ratio close to 1, the adaptive incrementally affine method offers highly accurate predictions; however, its accuracy is diminished with an increase in the reinforcement volume fraction or aspect ratio.

The complete details of the homogenization method can be found in our previous study [25, 26]; we provide some of these details herein for clarity. The yield reduction method reduces the yield stress of the matrix with the volume fraction of the reinforcement.

$$\sigma_y \leftarrow (1 - v_1)\sigma_y \text{ for the matrix} \quad (7)$$

The adaptive incrementally affine method for elasto-plastic composites is summarized as follows. Here, subscripts 0 and 1 represent variables of the matrix and reinforcement, respectively (e.g., $\mathbf{C}_0$ refers to the stiffness tensor of the matrix and $\mathbf{C}_1$ refers to the stiffness tensor of the reinforcement).

1. A macro-strain increment ($\Delta\bar{\epsilon}$) is applied to the composite for a given strain state at t_n .
2. The strain increment of the reinforcement is initialized as a macro-strain increment:

$$\langle \Delta\epsilon \rangle_{w_1} = \Delta\bar{\epsilon}$$

where $\langle \bullet \rangle_{w_0}$ and $\langle \bullet \rangle_{w_1}$ refer to the volume averages over the matrix and particles, respectively.

3. The strain increment of the matrix is calculated as follows:

$$\langle \Delta\epsilon \rangle_{w_0} = \frac{1}{v_0} (\Delta\bar{\epsilon} - v_1 \langle \Delta\epsilon \rangle_{w_1}). \quad (8)$$

4. Eshelby's tensor ($\mathbf{S}$) [1, 38] and the concentration tensors ($\mathbf{B}_1^\epsilon$, $\mathbf{A}_1^\epsilon$) are computed as follows:

$$\mathbf{B}_1^\epsilon = [\mathbf{I} + \mathbf{S} : (\mathbf{C}_0)^{-1} : (\mathbf{C}_1 - \mathbf{C}_0)]^{-1} \quad (9)$$

$$\mathbf{A}_1^\epsilon = \mathbf{B}_1^\epsilon : (v_0 \mathbf{I} + v_1 \mathbf{B}_1^\epsilon)^{-1} \quad (10)$$

where $\mathbf{I}$ is the fourth-order identity tensor.

5. The residual tensor ($\mathbf{R}$) is computed as follows:

$$\begin{aligned} \mathbf{R} = & \mathbf{A}_1^\epsilon : \Delta\bar{\epsilon} - \langle \Delta\epsilon \rangle_{w_1} \\ & + (\mathbf{A}_1^\epsilon - \mathbf{I}) : (\mathbf{C}_1 - \mathbf{C}_0)^{-1} : (\boldsymbol{\sigma}_1(t_{n+1}) - \mathbf{C}_1 : \boldsymbol{\epsilon}_1(t_{n+1}) - \boldsymbol{\sigma}_0(t_{n+1}) \\ & + \mathbf{C}_0 : \boldsymbol{\epsilon}_0(t_{n+1})) \\ & + (\mathbf{I} - \mathbf{A}_1^\epsilon) : (\mathbf{I} - \mathbf{B}_1^\epsilon)^{-1} : [\mathbf{B}_1^\epsilon : \mathbf{C}_0^{-1} : \boldsymbol{\sigma}_0(t_n) - \mathbf{C}_1^{-1} : \boldsymbol{\sigma}_1(t_n)] \end{aligned} \quad (11)$$

- 6-1. If $|\mathbf{R}| > \text{tolerance}$, step 3 is repeated with a new trial.

$$\langle \Delta \boldsymbol{\varepsilon} \rangle_{w_1} \leftarrow \langle \Delta \boldsymbol{\varepsilon} \rangle_{w_1} + \mathbf{R} \quad (12)$$

6-2. If $|\mathbf{R}| < \textit{tolerance}$, then step 7 is followed.

7. The macro stress increment ($\Delta \bar{\boldsymbol{\sigma}}$) and effective stiffness tensor ($\bar{\mathbf{C}}$) are obtained as follows:

$$\Delta \bar{\boldsymbol{\sigma}} = v_0 \mathbf{C}_0 : (\langle \Delta \boldsymbol{\varepsilon} \rangle_{w_0} - \Delta \boldsymbol{\varepsilon}_0^p) + v_1 \mathbf{C}_1 : (\langle \Delta \boldsymbol{\varepsilon} \rangle_{w_1} - \Delta \boldsymbol{\varepsilon}_1^p). \quad (13)$$

$$\bar{\mathbf{C}} = [v_0 \mathbf{C}_0 + v_1 \mathbf{C}_1 : \mathbf{B}_1^\varepsilon] : [v_0 \mathbf{I} + v_1 \mathbf{B}_1^\varepsilon]^{-1}. \quad (14)$$

8. Step 1 is repeated for the next strain increment.

Under a given reinforcement volume fraction, the prediction accuracy of the homogenization method decreases as the aspect ratio of an ellipsoidal particle increases; this is because the mutual interaction among reinforcements increases, which further violates the mean-field assumption. Additionally, the prediction provided by the homogenization method has another source of error for cylindrical fiber-reinforced composites because Eshelby's solution assumes an ellipsoidal shape for the reinforcement.

The FEM offers an accurate numerical evaluation of the internal stress distribution and yield inside a composite under mechanical loading, and the outcome from the FEM can be considered as a ground truth if the implementation and numerical method are carefully executed. We employed the commercial software ABAQUS [39] with the UMAT code for the FEM simulations in this study. FEM data were generated considering the RVE; the reinforcement was embedded into an FCC configuration, as shown in Fig. 2. The analysis was conducted using only one-eighth of the RVE under periodic boundary conditions (PBCs). Depending on the aspect ratio and volume fraction of the reinforcement, approximately 15,000 to 108,000 elements are required to ensure convergence.

The computational costs for the homogenization method and FEM for the analysis of the composite are compared in Fig. 3. Here, we consider composites containing reinforcements

with an aspect ratio of 10, while the other input parameters are randomly assigned. For analyzing 100 composites, the homogenization method requires 5.2 h of single-core computation, whereas the FEM needs 56.8 h of eight-core computation; thus, the FEM is 87.4 times more expensive than homogenization in terms of computational cost. Considering a variety of input parameter sets, the predictions provided by the adaptive incrementally affine method are compared with the FEM results for the ellipsoidal-particle/fiber-reinforced composite in Fig. S1 (see Supplementary Information). Predictions from the homogenization methods show notable errors when the aspect ratio of the reinforcement or volume fraction is large. Moreover, although the FEM results are considered as ground truth in this study, experimental data (which also account for the effects from various manufacturing defects) can be used in the transfer learning scheme as well; this is discussed in the following section.

3. Application of transfer learning

Transfer learning has been widely used to train a task-specific model effectively by utilizing a pre-trained model with a massive dataset. Transfer learning can achieve powerful predictive performance even with a small amount of task-specific data by fine-tuning a subset of layers of the pre-trained model while typically freezing the feature extraction layers. In this study, we first pre-trained a DNN model with sufficient homogenization data to enable this pre-trained model to capture the underlying mechanism determining the effective stress-strain relationship for idealized ellipsoidal particle-reinforced composites. We then used task-specific data (FEM data) to fine-tune the pre-trained model for predicting the stress-strain relationship for an ellipsoidal-particle/fiber-reinforced composite. For the fine-tuning procedure, unlike in typical transfer learning, we trained the task-specific model with FEM data using the parameters of the pre-trained model as the initial parameters, instead of freezing subset layers from the pre-

trained model. We found that freezing some subsets degrades the performance of the fine-tuned DNN. This is because the knowledge that we seek to transfer is not an abstract feature but rather the general input and output structural relationships that are believed to be embedded in the overall layer of the pre-trained model. As shown in Fig. S2, the pre-trained model represents the general structure of the stress-strain curves well (the outputs are concave and monotonic functions).

The overall workflow of the transfer-learning framework is illustrated in Fig. 1. The DNN was constructed and trained using Keras [40] on Python 3.7. We first generated 59,500 data using the homogenization method. We then constructed 2,000 data from computationally expensive FEM simulations. The homogenization data were divided into training and validation sets in a ratio of 49,000:10,500. The FEM data were divided into training, validation, and test sets in a ratio of 1,400:300:300. The validation set was used as an early stopping criterion for training the DNN, and the test set was used for assessing the model. Each input parameter listed in Table 1 is normalized to values between 0 and 1. The output data, i.e., the stress-strain curves evaluated at 101 strain points (i.e., the dimension of the output is 101), are compressed into 10-dimensional vectors comprising the 10 most important principal components extracted via principal component analysis (PCA), as depicted in Fig. 4 (a), according to a previously proposed scheme [15]. The cumulative explained variance, which is defined as the sum of eigenvalues normalized by the sum of all eigenvalues ($\sum_{i=1}^{10} \lambda_{ii} / \sum_{i=1}^{101} \lambda_{ii}$) is 99.999%. The data that are dimensionally reduced via PCA, i.e., the 10 most important principal components, are normalized to values between 0 and 1 for efficient training. We chose a DNN architecture, which does not impose any structural assumption (inductive biases), to employ as flexible a model as possible to express the complex stress-strain relationship of elasto-plastic composites. A dense layer, batch normalization, and activation function

constitute a unit layer in the DNN architecture as shown in Fig. 4 (b). Batch normalization is known to accelerate training, mitigate the sensitivity to initial weights, and have a regularization effect [41, 42]. The weighted mean squared error (WMSE) is defined for DNN training as follows:

$$\text{WMSE} = \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^{10} \sqrt{\lambda_{jj}} (Y_{j,i}^{\text{true}} - Y_{j,i}^{\text{pred}})^2 \quad (15)$$

where $Y_{j,i}$ refers to the j -th principal component of the i -th sample, λ_{jj} refers to the j -th eigenvalue, and n refers to the number of samples. The variation between eigenvalues is exceedingly high; hence, the squared eigenvalues are used as weights. To optimize the DNN architecture, grid-search hyper-parameter tuning is performed to search for the best combination of the number of unit layers, the number of neurons in each layer, and the type of activation function [43-45]. We chose the architecture with the lowest average error after five epochs in the following search space (see Supplementary Note 1).

Number of neurons of each layer = [40, 50, 60, 70, 80, 90, 100, 110, 120]

Number of hidden unit layers = [3, 4, 5, 6, 7]

Activation function = [ReLU, GeLU, ELU, LeakyReLU]

The best architecture has 50 neurons for each layer, six hidden unit layers, and exponential linear unit (ELU) as an activation function as shown in Fig. 4 (b); this leads to 14,010 trainable parameters. The Adam optimizer, an adaptive learning rate optimizer, was used for training [46]. The batch size was set to one-tenth of the training dataset size. After each epoch, the training dataset was randomly shuffled to minimize the sample bias. As depicted in Fig. 1, Model A was trained using sufficient homogenization data with a low computational cost. Taking the weights of Model A as the initial weights, Model B was fine-tuned using only a few FEM data, which entailed a relatively high computational cost. Then, based on the trained

model, 101-dimensional stress-strain curves were recovered from 10-dimensional principal component arrays via reverse normalization and reverse PCA. Hereinafter, Model A refers to a DNN model trained with homogenization data, Model B represents a DNN model trained via transfer learning based on both homogenization data and FEM data, and Model C indicates a DNN model trained only with FEM data.

Neural networks must have sufficient width, depth, and trainable parameters when the relationship between the input and output is complex. In such circumstances, a large amount of data is required for the DNN to achieve satisfactory generalization performance (i.e., prediction of unseen data). Training with a small amount of data would lead to an over-fitted model with poor generalization. The transfer learning strategy proposed in this study is illustrated in Fig. 5. The x -axis represents how general knowledge is extracted from the abundant homogenization data through pre-training. Owing to the abundance of the homogenization data, the pre-trained model becomes sufficiently general to serve as a structural foundation for various task-specific models. The y -axis represents how the pre-trained model is fine-tuned using FEM data to form task-specific models. Model C suffers from overfitting owing to the lack of data, especially when using a flexible DNN architecture. Meanwhile, Model A cannot accurately predict the task-specific stress-strain relationship of composites, because of the limitation of the homogenization theory. Despite the difference between the predictions provided by homogenization and the FEM, these predictions share the underlying mechanism determining the effective stress-strain relationship. We believe that Model A captures the underlying mechanism based on the homogenization theory. Relying on the general stress-strain relationships extracted from the pre-trained model, Model B can be quickly adapted for ellipsoidal-particle/fiber-reinforced composites, avoiding overfitting, even when using a small amount of task-specific FEM data. In summary, we used a large volume of

low-fidelity data to train a general and sufficiently large DNN model to extract the structural relationships between the stress and strain of idealized composites. We then fine-tuned the pre-trained model to increase the predictive accuracy using few but high-fidelity FEM data.

4. Result and discussion

We used the DNN trained via transfer learning to predict the stress-strain curves of elastoplastic composites. To evaluate the performance of transfer learning, the DNN model trained via transfer learning using both homogenization and FEM datasets was compared with the DNN model trained only with a small FEM dataset. The DNN architectures and initial weights of the two models were identical. In addition, we used the same training, validation, and test datasets from the FEM for both DNN models.

4.1. Ellipsoidal particle reinforced composite

We considered an ellipsoidal particle-reinforced composite subjected to uniaxial tensile loading. FEM data were generated using an RVE with reinforcement particles in the FCC configuration as shown in Fig. 2 (a, b). The prediction and ground truth of the top three principal components are compared between Models B and C in Fig. 6, which clearly shows that transfer learning is superior to direct training in predicting principal components. The R^2 values, which are statistical measurements representing how closely the regression fits the data, were much higher in Model B, as indicated in Table 2. In Model B, the R^2 values from transfer learning were remarkably high across all 10 principal components, while in Model C, the R^2 values decreased significantly for less important principal components. The maximum error of each stress-strain curve is defined as follows:

$$\text{Maximum Error} = \max\left(\frac{\sigma_1^{Pred} - \sigma_1^{FEM}}{\sigma_1^{FEM}}, \dots, \frac{\sigma_{101}^{Pred} - \sigma_{101}^{FEM}}{\sigma_{101}^{FEM}}\right). \quad (16)$$

The maximum error histogram is presented for 300 test data in Fig. 7. Model B, trained via transfer learning, outperformed Model C, which was directly trained with the FEM dataset. The predictions from both models are presented in Fig. 8 for the four cases in which model C exhibited the greatest errors. Transfer learning shows reliable predictions even for the worst cases. Moreover, Fig. S2 presents the four worst cases in which Model A, the DNN trained only with the homogenization dataset, exhibited the greatest errors (see Supplementary Information). The comparison between the results from Models A and B clearly shows that the DNN pre-trained with the homogenization dataset is fine-tuned appropriately via transfer learning.

4.2. Fiber-reinforced composite

Homogenization theories based on Eshelby's solution assume that reinforcements are ellipsoidal. In this section, we verify whether transfer learning using homogenization data can be applied to a composite containing non-ellipsoidal reinforcements. The homogenization method has frequently been used to analyze composites having cylindrical or disk-shaped reinforcements with high aspect ratios [47, 48]. In the present study, an FEA was performed on the FCC-structured RVE of a cylindrical fiber-reinforced composite, as shown in Fig. 2 (c, d). We generated 2,000 FEM data and divided them into training, validation, and test sets in a ratio of 1,400:300:300. The same homogenization dataset as that mentioned in Section 4.1 was used for transfer learning, that is, the DNN pre-trained by the homogenization dataset, where the ellipsoidal reinforcement was assumed, was fine-tuned with the FEM dataset on composites containing cylindrical fiber reinforcements. The maximum error histogram for the 300 test data is shown in Fig. 9. The predictions from both models are presented in Fig. 10 for the four cases

in which Model C exhibited the greatest errors. Fig. S3 shows the predictions for the four cases in which Model A exhibited the greatest errors (see supplementary information). As described in Section 4.1, Model B, trained via transfer learning, achieved the best predictive performance. These results confirm that transfer learning with homogenization data can also be applied to composites embedded with non-ellipsoidal reinforcements. For example, for composites containing flake-like reinforcements, such as graphene platelets, a DNN can be pre-trained using homogenization data generated by assuming oblate spheroid particle reinforcements; the DNN can then be fine-tuned with FEM data or experimental data via transfer learning.

5. Conclusion

In this study, we demonstrated a transfer learning-based composite analysis technique that can efficiently exploit a large dataset based on the homogenization method when only a small dataset from FEM simulations or experiments is available because of high computational and economic costs. Because machine learning is a data-hungry technique, better generalization can be achieved with a greater amount of data. The homogenization theory has the advantage of providing a large amount of data at a lower cost and within a shorter time compared with the FEM or experimental methods, although its prediction accuracy is relatively inferior. Considering the task of predicting the elasto-plastic response of particle/fiber-reinforced composites, we demonstrated that the accuracy and efficiency of a composite analysis can be improved by training a DNN model with a large but less accurate dataset based on the homogenization method and then fine-tuning the DNN with an accurate but small dataset based on the FEM. Although we adopted the adaptive incrementally affine method to generate the homogenization data, several other homogenization theories can also be applied to the initial training dataset in the transfer learning scheme. The proposed method can easily be generalized

to enable accurate and efficient prediction of various properties of composites with only a small, accurate dataset when any of the homogenization theories can determine the qualitative features of the composite.

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Tables

Table 1. Input parameters with given ranges for elasto-plastic composites.

ν_0	σ_y/E_0	k/E_0	n	E_1/E_0	ν_1	AR	f_1
0.1~0.45	0.005~0.025	0.01~0.1	0.2~0.6	1~200	0.1~0.45	1~10	1%~30%

Table 2. Comparison of R^2 values for 10 principal components from Model B (transfer learning) and Model C (DNN with FEM)

	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th
Model B	0.999	0.995	0.997	0.988	0.990	0.980	0.986	0.970	0.960	0.948
Model C	0.991	0.985	0.976	0.904	0.787	0.471	0.317	0.317	0.187	0.045

Figures and captions

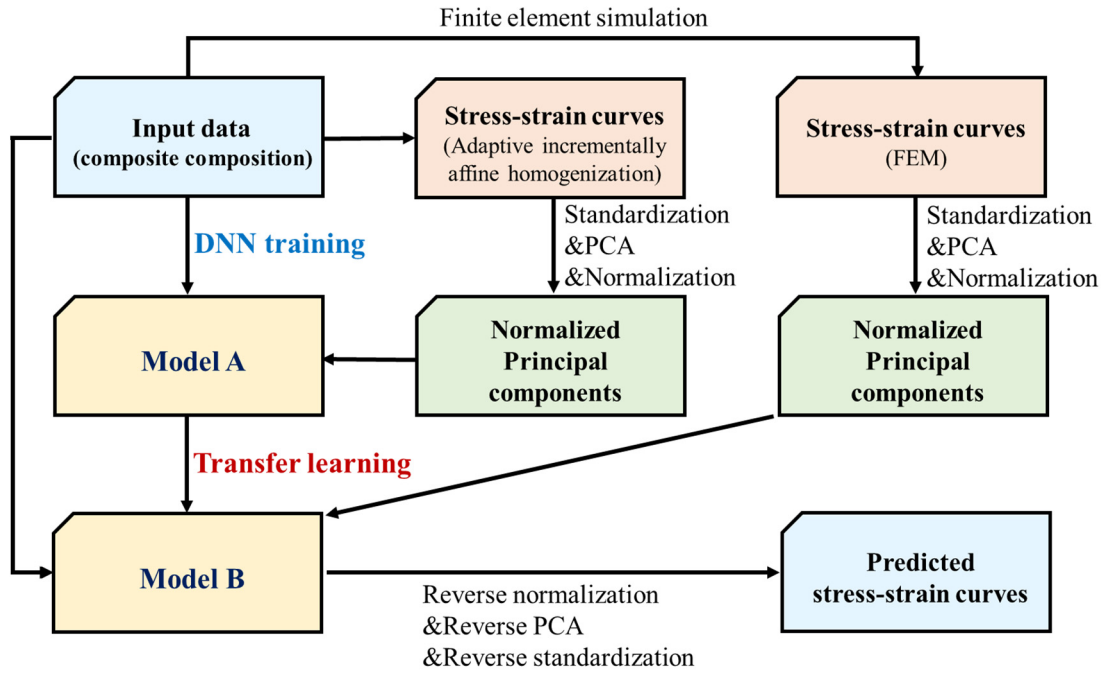


Fig. 1. The overall workflow for transfer learning. Model A was trained using a significantly large homogenization dataset at a low computational cost. Applying transfer learning, Model B was fine-tuned with a relatively small FEM dataset using Model A as a starting point. Model C refers to the model trained only based on the FEM dataset. To verify the superiority of transfer learning approach, the performances of models B and C were compared.

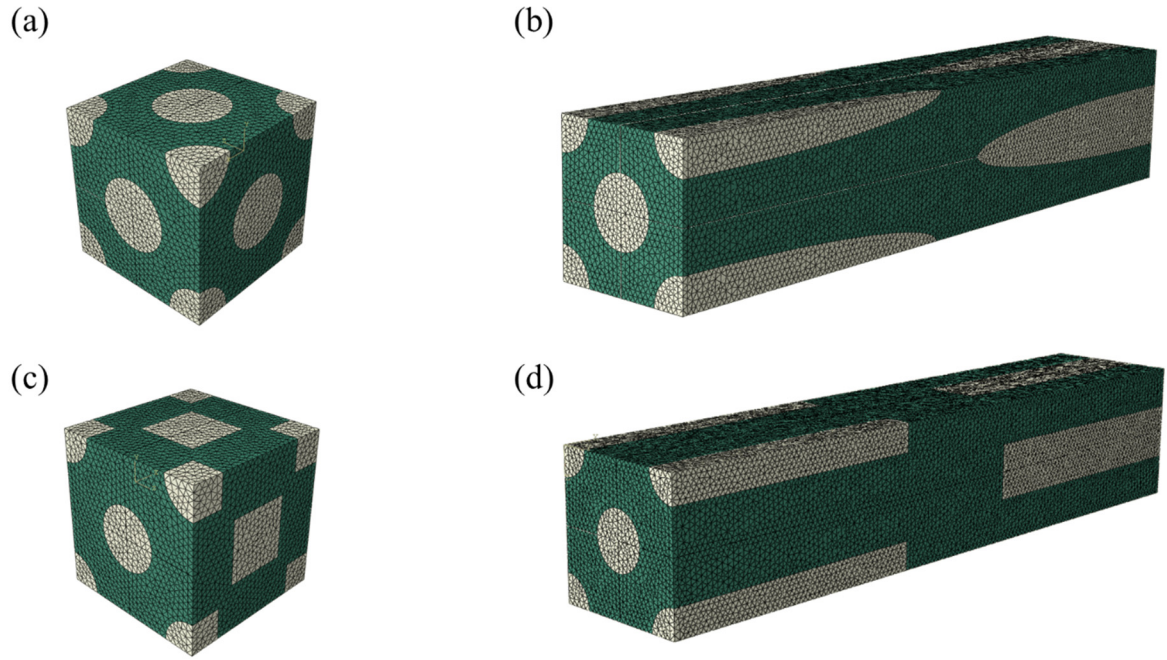


Fig. 2. FCC-structured RVE for FEM. (a, b) Spherical particle and ellipsoidal particle-reinforced composite, respectively. (c, d) Composite containing fiber-reinforcements with aspect ratios of 1 and 10, respectively. (b, d) Half of FCC unit cell structure. Volume fractions of reinforcements are 20%.

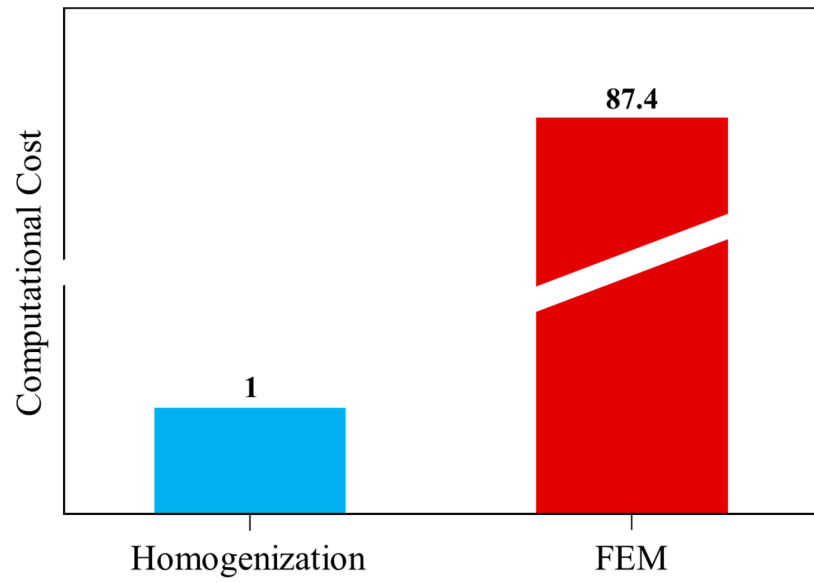


Fig. 3. Comparison of computational cost between homogenization method and FEM. The computational cost was defined by multiplying the computational time by the number of cores used in the simulation.

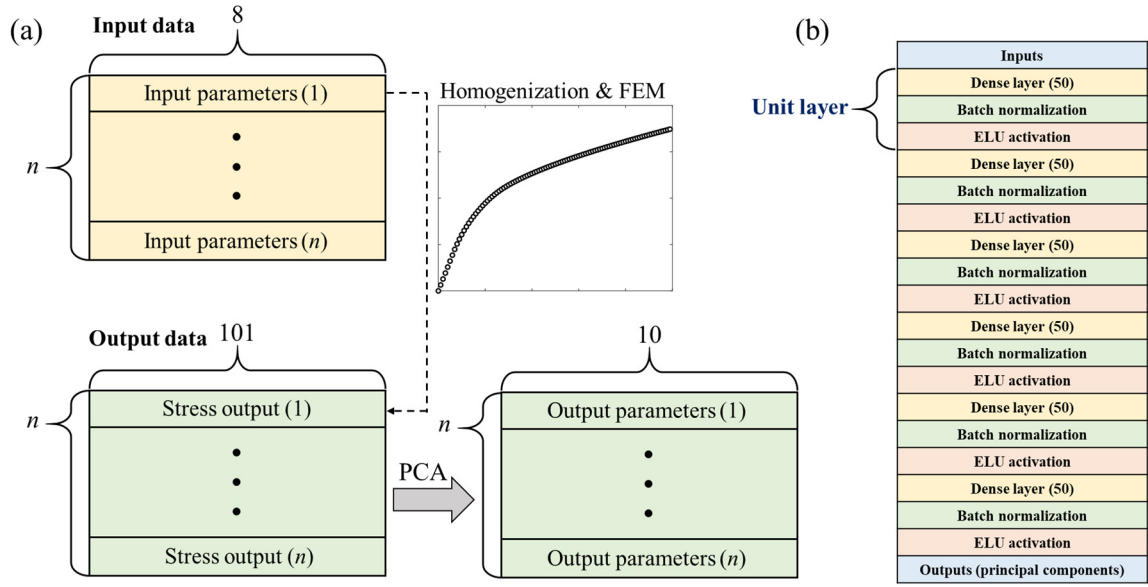


Fig. 4. (a) Data format of input (composite composition) and output stress-strain curve data). 101-dimensional stress data was compressed into 10-dimensional data via PCA. (b) DNN architecture was composed of six unit layers.

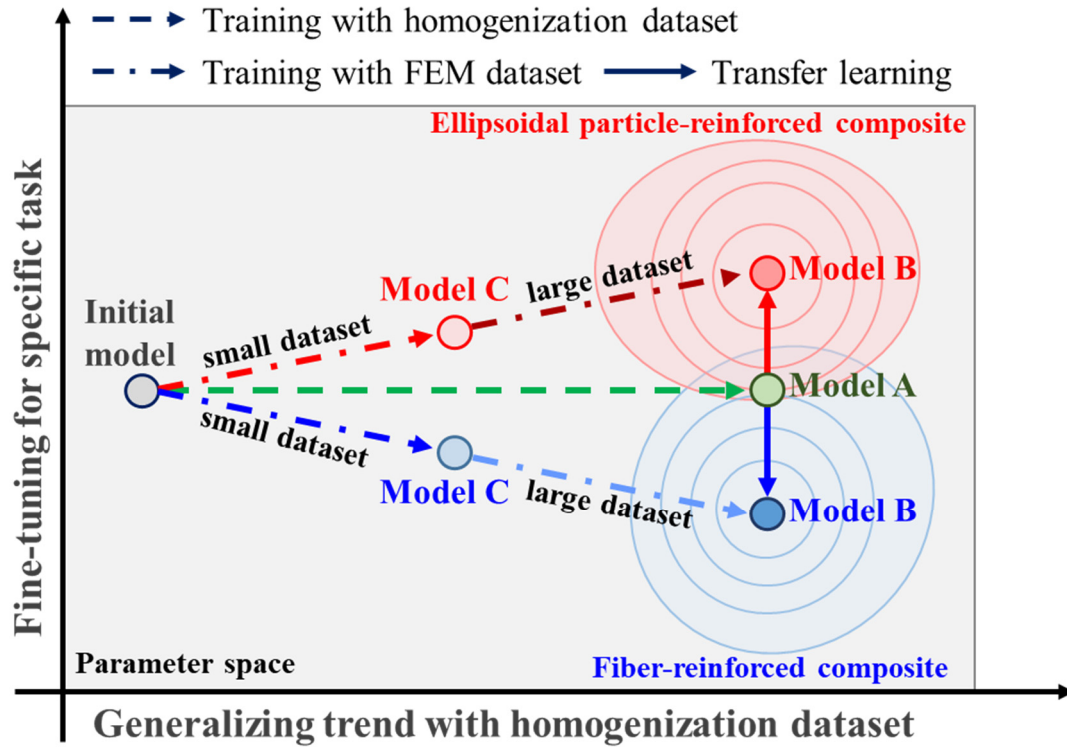


Fig. 5. Schematic of how transfer learning shows better performance. The initial model was set with random weights. Pre-training with a large homogenization dataset allowed DNN to capture the underlying mechanism between input and output. The transfer learning enabled the model to be fine-tuned from Model A based on homogenization theory. Model C suffered from overfitting owing to a lack of data.

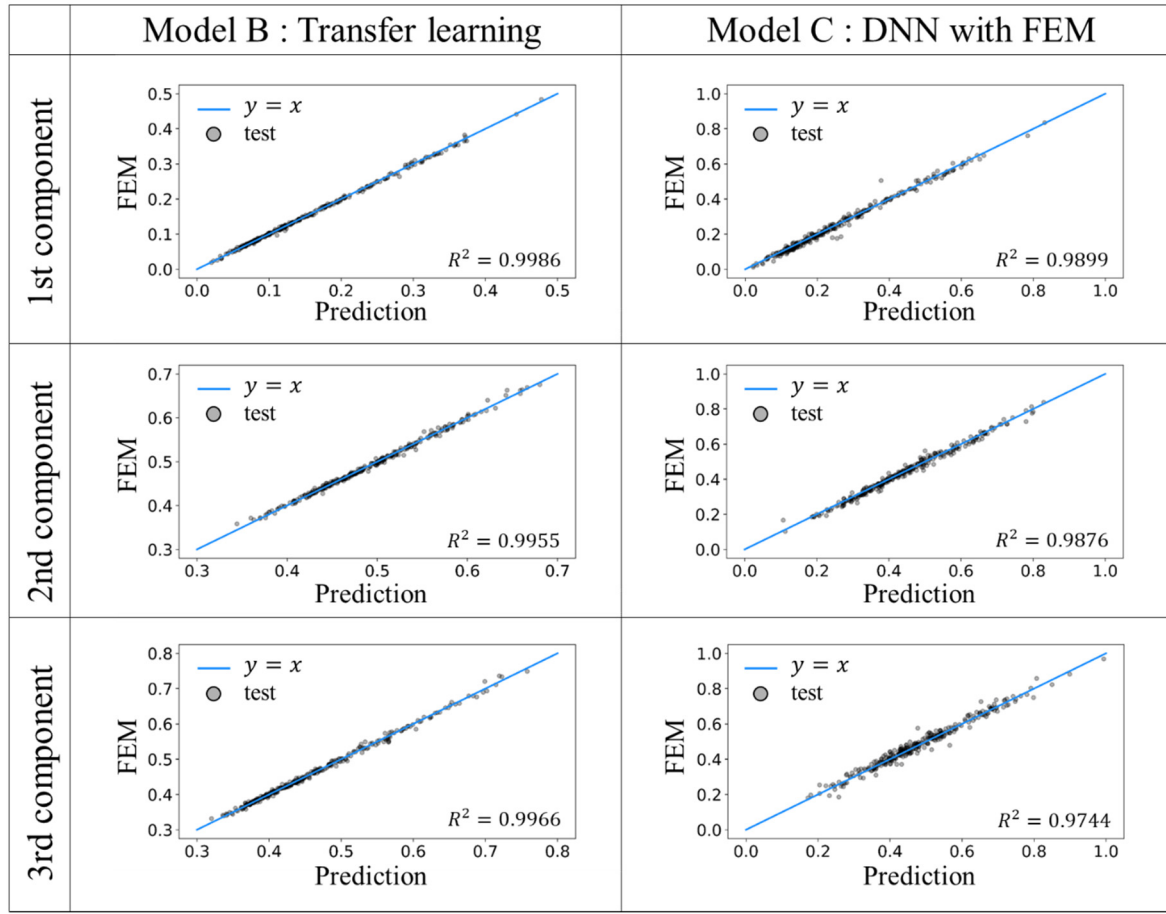


Fig. 6. Comparison between prediction (transfer learning/DNN with FEM) and ground truth (FEM) of the top three principal components. Model B refers to the model applying transfer learning. Model C refers to the model trained only with FEM data. 300 test data were used for comparison.

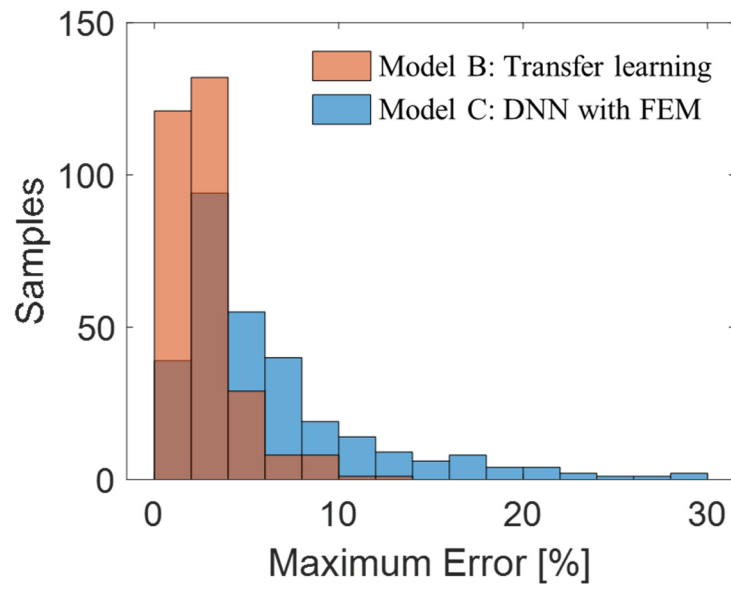


Fig. 7. Comparison between performances of transfer learning and DNN with FEM for ellipsoidal particle-reinforced composite. The error was defined as maximum relative error for each stress-strain curve prediction compared to ground truth (FEM). 300 test data were used for comparison.

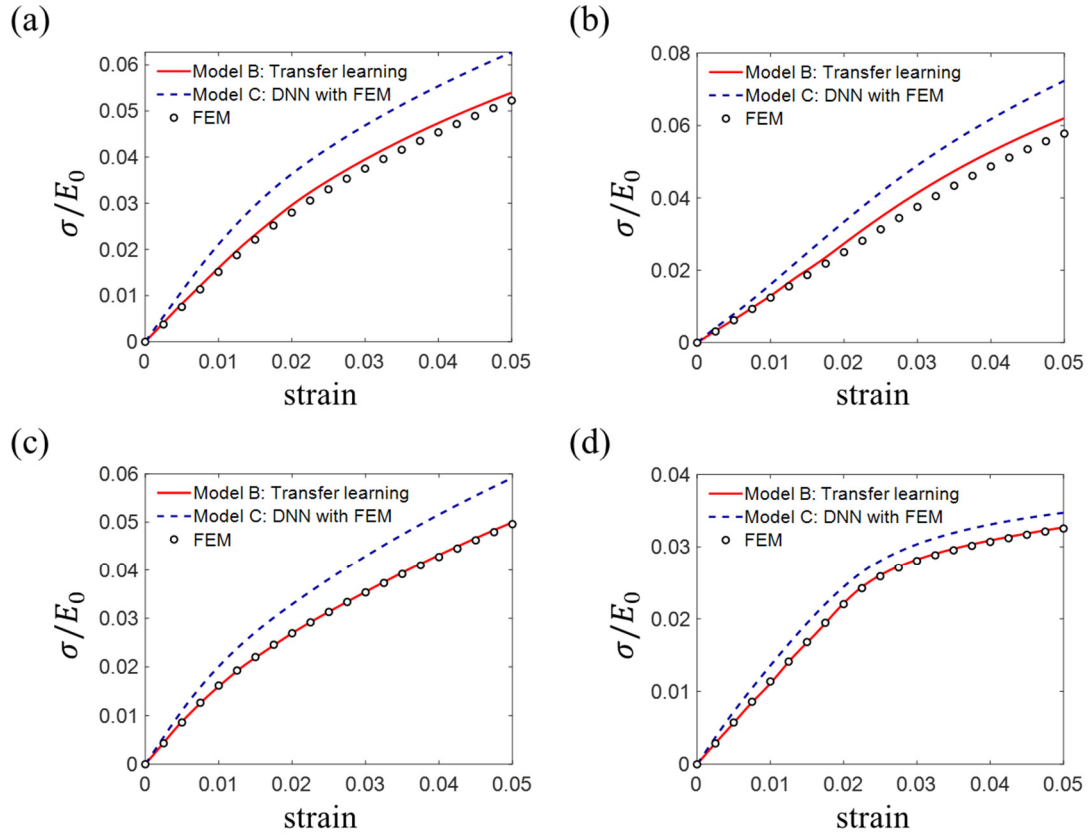


Fig. 8. Comparison between prediction (transfer learning/DNN with FEM) and ground truth (FEM) where DNN with FEM exhibited the top four maximum relative errors for ellipsoidal particle-reinforced composite.

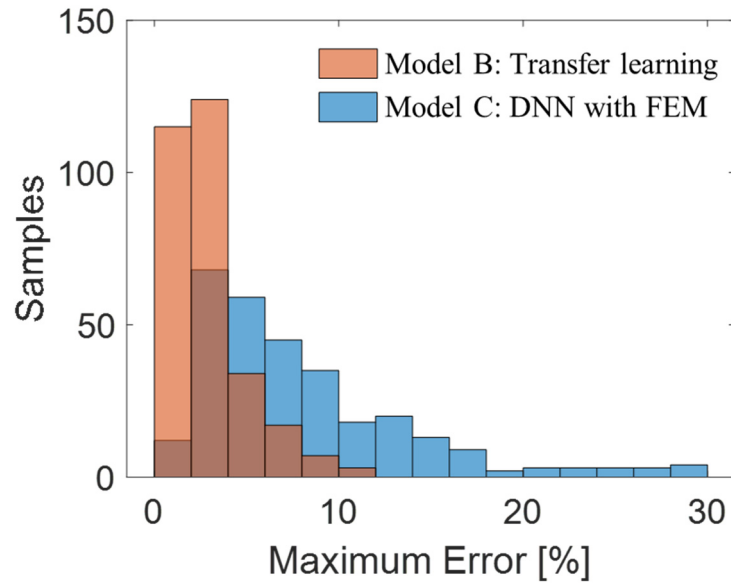


Fig. 9. Comparison between performances of transfer learning and DNN with FEM for fiber-reinforced composite. The error was defined as maximum relative error for each stress-strain curve prediction compared to ground truth (FEM). 300 test data were used for comparison.

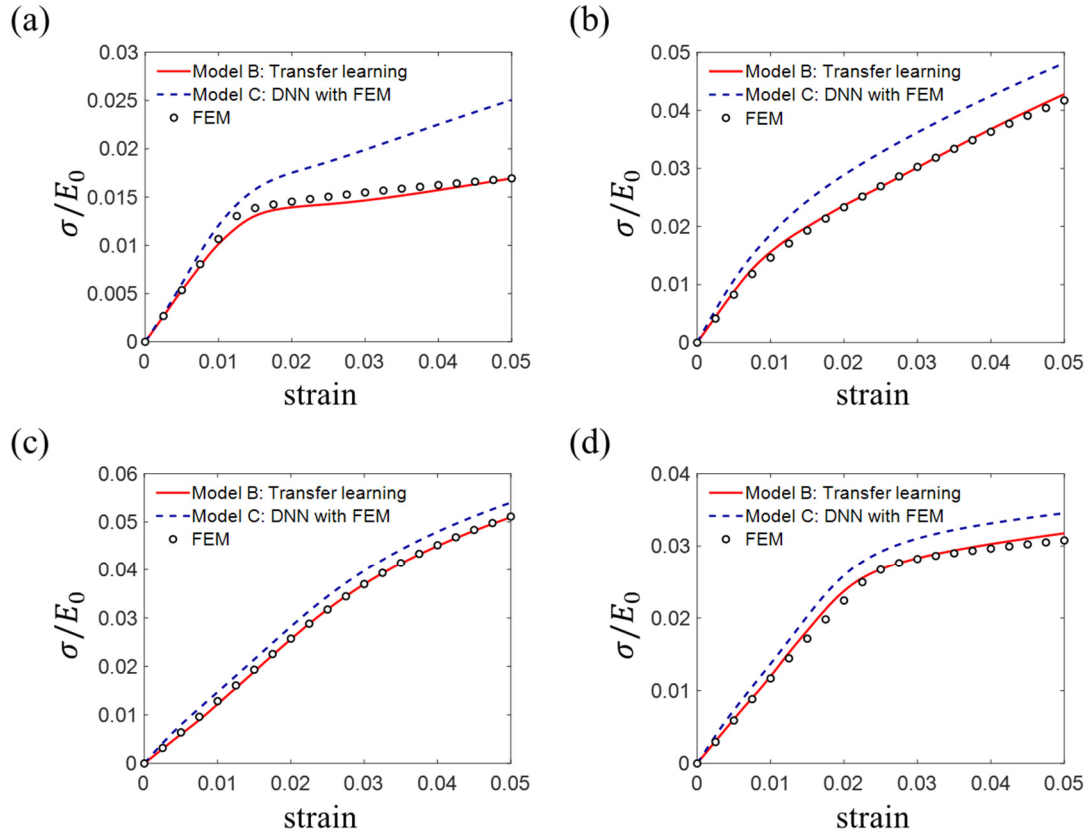


Fig. 10. Comparison between prediction (transfer learning/DNN with FEM) and ground truth (FEM) where DNN with FEM exhibited the top four maximum relative errors for fiber-reinforced composite.

Supplementary information

Transfer learning for enhancing the homogenization-theory-based prediction of elasto-plastic response of particle/fiber-reinforced composites

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Keywords

Homogenization, Transfer learning, Adaptive incrementally affine, Fiber-reinforced composite, Machine learning, Deep Neural Network

Supplementary Note 1: Grid-search technique for an optimized architecture of DNN.

The grid-search hyper-parameter tuning technique was used to find the optimal architecture of DNN. The number of neurons, number of hidden unit layers, and types of activation function were investigated as follows,

Number of neurons of each layer= [40, 50, 60, 70, 80, 90, 100, 110, 120]

Number of hidden unit layers = [3, 4, 5, 6, 7]

Activation function = [ReLU, GeLU, ELU, LeakyReLU]

The average Weighted Mean squared errors (WMSEs) after five epochs were obtained over 50 iterations with random initial weights.

Table S1. WMSE results with ReLU activation function. The training epoch was set to be five.

The minimum value is shaded.

		Number of hidden unit layers				
		3	4	5	6	7
Number of neurons	40	0.021048	0.018229	0.017952	0.016734	0.016384
	50	0.021257	0.018585	0.018039	0.015661	0.015427
	60	0.020385	0.018528	0.016343	0.01608	0.01469
	70	0.020767	0.019605	0.016729	0.015563	0.015256
	80	0.020744	0.019068	0.016572	0.015065	0.015291
	90	0.020769	0.018474	0.017576	0.015486	0.014907
	100	0.020519	0.019465	0.016383	0.016704	0.015012
	110	0.021459	0.020514	0.017766	0.015972	0.015501
	120	0.021291	0.019835	0.01802	0.016883	0.014938

Table S2. WMSE results with GeLU activation function. The training epoch was set to be five.
The minimum value is shaded.

		Number of hidden unit layers				
		3	4	5	6	7
Number of neurons	40	0.013834	0.012969	0.012673	0.012321	0.012993
	50	0.013717	0.012541	0.01216	0.01202	0.013457
	60	0.013649	0.013089	0.012377	0.01226	0.013448
	70	0.013765	0.013177	0.012696	0.012593	0.012944
	80	0.013793	0.013343	0.012853	0.013135	0.013324
	90	0.014331	0.013983	0.013407	0.013001	0.013216
	100	0.014532	0.01421	0.013574	0.013126	0.013062
	110	0.01447	0.014512	0.013494	0.013318	0.013778
	120	0.014834	0.014721	0.013615	0.013719	0.014059

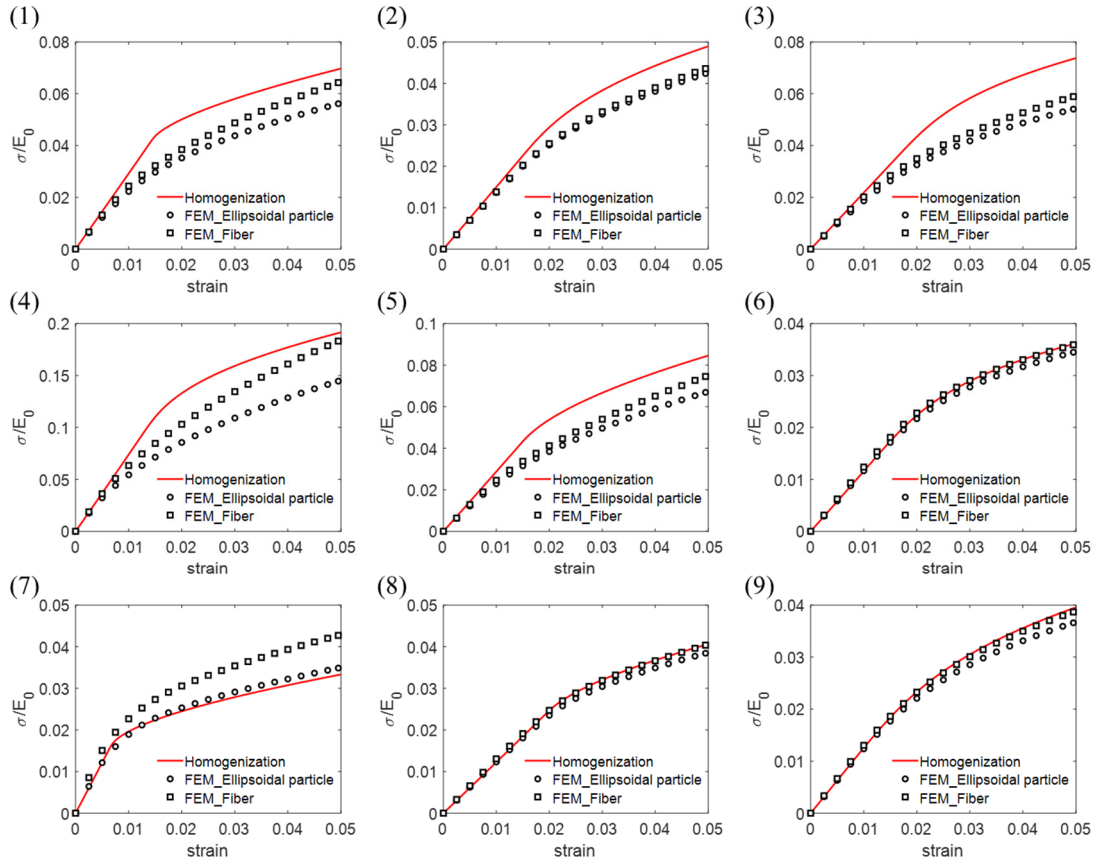
Table S3. WMSE results with ELU activation function. The training epoch was set to be five.
The minimum value is shaded.

		Number of hidden unit layers				
		3	4	5	6	7
Number of neurons	40	0.013316	0.011389	0.011121	0.010042	0.010741
	50	0.012655	0.011312	0.010672	0.01004	0.010713
	60	0.011649	0.011444	0.010717	0.0105	0.010093
	70	0.012533	0.010945	0.011042	0.011174	0.010737
	80	0.012648	0.011381	0.011442	0.010653	0.010547
	90	0.012682	0.011546	0.0111	0.010933	0.010814
	100	0.011827	0.011751	0.011254	0.011521	0.01155
	110	0.012861	0.011959	0.011675	0.011598	0.011877
	120	0.012581	0.011975	0.011388	0.011807	0.012063

Table S4. WMSE results with LeakyReLU activation function. The training epoch was set to be five. The minimum value is shaded.

		Number of hidden unit layers				
		3	4	5	6	7
Number of neurons	40	0.019277	0.018135	0.016184	0.015526	0.015434
	50	0.019117	0.017132	0.015867	0.015625	0.015056
	60	0.019048	0.016921	0.016675	0.014842	0.015097
	70	0.018252	0.017961	0.016616	0.015567	0.014759
	80	0.018704	0.018388	0.017224	0.015154	0.014992
	90	0.019169	0.018324	0.01731	0.015871	0.015361
	100	0.019628	0.018246	0.017708	0.016168	0.015017
	110	0.019627	0.018332	0.017221	0.015854	0.014715
	120	0.019449	0.018953	0.016989	0.016308	0.015456

Supplementary Figures and captions



	v_0	E_1/E_0	v_1	f_1	σ_y	κ	n	AR
1	0.29697	166.4253	0.329579	0.11756	0.01813	0.067332	0.561568	7.731474
2	0.146601	29.97139	0.274128	0.040192	0.016046	0.073401	0.368099	8.674419
3	0.105324	194.1244	0.330702	0.10308	0.019568	0.064213	0.299783	5.369895
4	0.357501	138.656	0.421726	0.266517	0.021927	0.053083	0.359545	9.629458
5	0.236702	65.35032	0.41488	0.138538	0.019334	0.092898	0.490097	7.130942
6	0.43551	121.4034	0.104713	0.033438	0.010294	0.054976	0.246899	2.716982
7	0.144973	184.6046	0.322541	0.29363	0.01314	0.044156	0.523627	2.042282
8	0.387649	146.7278	0.137888	0.029631	0.020899	0.093473	0.503418	4.400982
9	0.253365	78.48515	0.19658	0.046314	0.00556	0.072156	0.257396	3.34039

Fig. S1. Homogenization predictions (solid lines) are compared to FEM results for ellipsoidal particle-reinforced composite (circular symbols) and fiber-reinforced composite (square symbols).

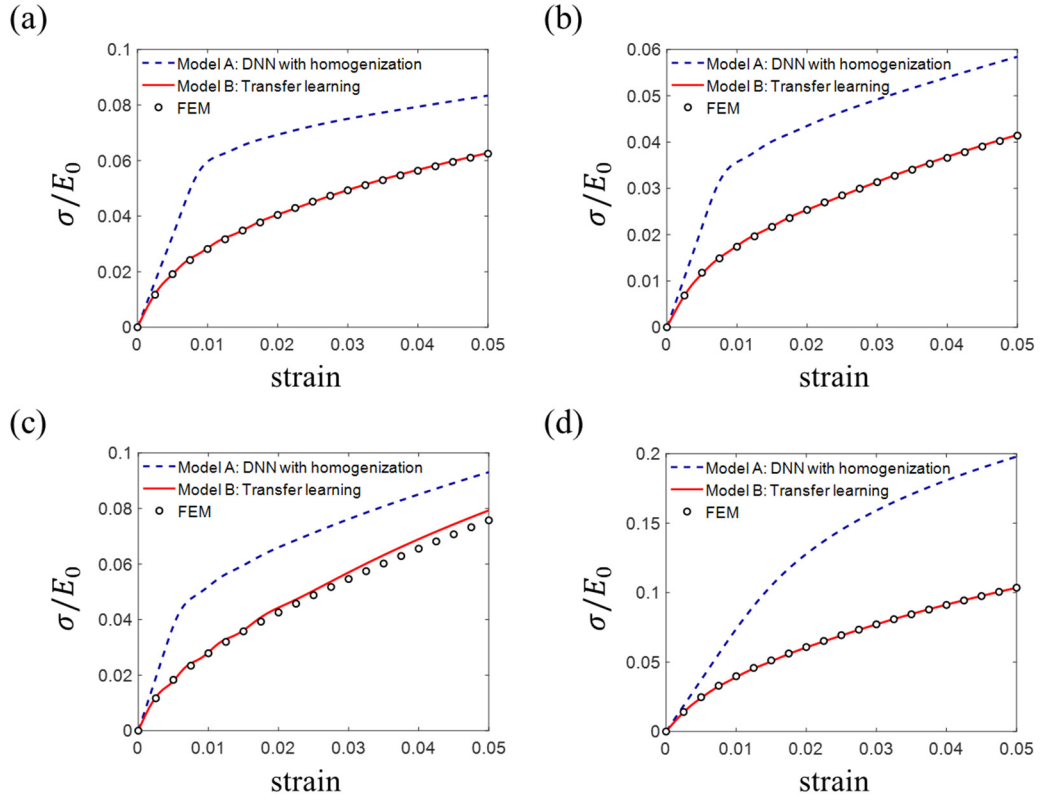


Fig. S2. Comparison between prediction (transfer learning/DNN with homogenization) and ground truth (FEM) where DNN with homogenization exhibited the top four maximum relative errors for ellipsoidal particle-reinforced composite. Model A refers to the model trained only with homogenization data. Model B refers to the model applying transfer learning.

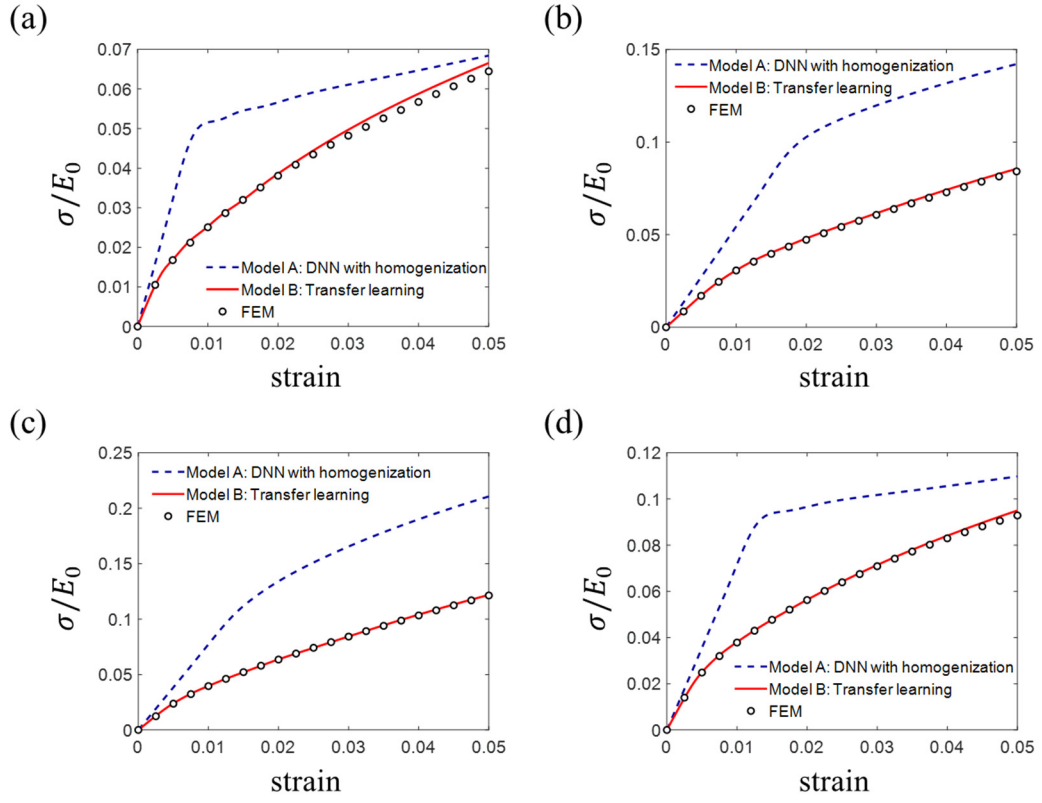


Fig. S3. Comparison between prediction (transfer learning/DNN with homogenization) and ground truth (FEM) where DNN with homogenization exhibited the top four maximum relative errors for fiber-reinforced composite. Model A refers to the model trained only with homogenization data. Model B refers to the model applying transfer learning.