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Research Article

A Data-driven Multiscale Analysis by Combination of Cluster-based Non-uniform Transformation Field Analysis and Artificial Neural Network

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Abstract

Data-driven computational mechanics have been used in the field of multiscale analysis where the constitutive modeling of composites is obtained by learning the material database obtained experimentally or numerically, using artificial neural network (ANN). In this paper, we present a data-driven multiscale analysis by combining the cluster-based non-uniform transformation field analysis (CNTFA), a reduced order model for the numerical homogenization of composites with periodically arranged microstructure, with ANN. Here, the CNTFA which was developed by the authors is efficient reduced order model for multiscale analysis of different nonlinear composites. Feed-forward neural network, a neural network is designed and trained for calculating the material stiffness and reproducing the microscale field quantities. The stiffness of homogenized material is approximately calculated using the gradient of ANN and strain concentration tensor. The proposed method can be effectively used in reproduction of field information (e.g. strain and stress) at the microscale as well as the analysis of structures at the macroscale. This property is distinguished with other cluster based methods such as SCA, VCA, FCA, in which the field information is reproduced at cluster level, not microscale level. An example calculation of three-point bending beam shows that the proposed method is very effective for the multiscale analysis of nonlinear composite structures.

Keywords

ANN, Data-driven Computational Mechanics, Cluster-based Non-uniform Transformation Field Analysis, Reproduction

1. Introduction

According to the development of the composites with excellent mechanical performances as well rapid improvement of computer performances, a number of new modeling techniques are developing in the field of computational mechanics. In general, it is said that the material constitutive models are the core of computational mechanics. Starting from the classical constitutive model that expresses mathematically material's behavior through a simple experiments such as Lamberg-Osgood hardening model [1], better constitutive models have been developed based on the comprehensive theories such as the non-associative flaw rules, the thermo-mechanics and the damage mechanics: rock model [2], soil

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model [3], plastic model [4], viscoelastic constitutive model [5]. In the studies of these models, the authors try to find the proper function formula which reveal the constitutive relation of given materials and decide the material parameters by performing the several experiments.

Unlikely the classical constitutive models, since the beginning of 1990s, many neural network (NN)-based material constitutive models have been developed by introducing the ANN to the field of computational mechanics [6-9]. NN-based material constitutive models are quite distinctive from previous others. In the previous modeling, the constitutive relations can be only obtained by combining comprehensive mechanical theories with experiments. Also, in the case of highly nonlinear interactions, it is almost impossible to find the proper constitutive relation by using this modeling. However, the NN-based modeling needs no any complex theories and assumptions, and it can be used by developing all the constitutive relations with any complex nonlinearity. Furthermore, it is possible to calculate the material stiffness [8].

The NN-based modeling also plays an important role in the studies of multiscale analysis of composite structure. In general, high performance composites commonly reveal various nonlinearities and have their complicated structures, so excellent numerical techniques are needed in order to predict the material characteristics. With the development of both the homogenization theory and the multiscale theory, there was a lot of progresses in the studies to predict effective responses of composites. Particularly, in the homogenization theory, the reduced order models are successively developed to predict the effective behavior of representative volume element (RVE) of composites at high accuracy by low cost. The developed models are: TFA [10], NTFA [11], RNEXP [12], SCA [13], VCA [14], FCA [15], and CNTFA [16]. Of which, SCA, FCA, VCA and CNTFA, as the reduced order models, are especially interesting in the field of multiscale theory because they use the cluster discretization technique that is being recognized as an effective data compressing method in the information engineering. Above all, the CNTFA allows to achieve a high calculation effectiveness, performing both the basis reduction by proper orthogonal decomposition and the reduction of degree of freedom by the clustering method. Afterward, CNTFA is successfully applied to the nonlinear issues: viscoelastic material [17] and anisotropic material [18]. These reduced order models have the two characteristics: to effectively predict the effective behavior and to reproduce the microscopic field information of RVE. In ref. [19], it was shown that the SCA has the ability not only to predict the effective behavior, but also to reproduce the cluster-wise mesoscopic field information. On the other hand, in ref. [18], the authors found that microscopic field information at the integral point can be reproduced even in the woven composites which possess crimp regions with complicated local strain distribution by using CNTFA. Unfortunately, despite of these advances in the studies of reduced order models, no effective method has been yet developed to obtain the effective material constitutive model with the calculating the stiffness of composite materials. This was not unsolved until the combination of reduced order models with NN- based models, and the data-driven multiscale analysis has been developed as a new field of the computational mechanics [20].

In the data-driven multiscale analysis, it is possible to calculate the effective behavior and material stiffness of homogenized composites by directly using NN-based constitutive modeling on the material database generated by using reduced order model. In recent, the cluster-based reduced order models such as SCA, VCA, FCA are combined with the theories of damage and fracture mechanic, so effective data-driven multiscale methods applicable to various structural issues are being developed [20]. In ref. [19], authors summarized the cluster-based reduced order models - SCA, VCA, FCA and described the generalized methodology of data-driven computational mechanics consisting of two stages, i.e., a stage of reduced order model and a deterministic stage for predicted value. Also, in ref. [21], the authors summarized the data-driven multiscale modeling and its applications using NN-based models, with further problems to be solved. Of which, one is to solve the problem such that a lot of computational time is consumed in generating the learning data necessary to ANN. To solve this, there are two possibilities:

a) Expanding the generated material database quantitatively as like in ref. [22], which the one for the isotropic material is expanded by using the permutation. A universal methodology, however, should be found even for the anisotropic materials.
b) Reducing the size of necessary learning data by composing the physics-based NN as like in ref. [23]. Here, it is essential to define the loss function by using the physical laws.

Nevertheless, in spite of these problems, the data-driven multiscale analysis is effectively used in practical issues at structural levels: topology optimization [19], fiber-reinforced composite plate analysis [24], and composite cutting process [25].

In this paper, we propose a data-driven multiscale analysis using CNTFA as the reduced order model developed in previous ref. [16]. Here, in order to well-reflect the mechanical characteristics of nonlinear materials, we present a method to prepare the learning data unlikely the previous one in which a strain-stress paired data is used.

This paper is organized as follows: Section 2 gives a summary of reduced order model CNTFA. Section 3 deals with a creation of learning data using CNTFA and a learning methods of ANN. Section 4 shows computational examples for a three-point bending beam under bending stress. Finally, Section 5 concludes the paper.

2. A Review of Cluster-based Non-uniform Transformation Field Analysis (CNTFA)

First of all, the homogenization must be carried out for a structural analysis of composites with periodically-arranged RVEs. In this Section, we describe CNTFA, a reduced order model, which allows to predict an effective response of RVE consisted of several constituents at high accuracy.

To distinguish field information at different scales, promise the following notation: a field amount with superscript " ¯ " represent the quantity at the macroscale (structural level), another one without any superscript represent the quantity at the microscale (material point or integral point level). Then the following relation holds:

$$\bar{\sigma}(t) = \frac{1}{|\Omega|}\int_{\Omega} \sigma(x,t)d\Omega \tag{1}$$

$$\bar{\varepsilon}(t) = \frac{1}{|\Omega|}\int_{\Omega} \varepsilon(x,t)d\Omega \tag{2}$$

In general, the basic equation of RVE with periodic boundary condition are represented by the following boundary value problem:

$$\begin{cases} div\sigma(x,t) = 0 \; \forall x \in \Omega \\ \sigma(x,t) = C(x){:}\left(\varepsilon(x,t) - \varepsilon^p(x,t)\right) \forall x \in \Omega \\ \langle \varepsilon(x,t) \rangle = \bar{\varepsilon}(t) \\ PBC \end{cases} \tag{3}$$

Here, σ, ε and ε^p are the vectors of stress, strain and plastic strain at the microscale respectively, and $\bar{\varepsilon}(t)$ is a vector of strain at the macroscale. PBC means a periodical boundary condition.

Suppose that a plastic strain field $\varepsilon^p(x,t)$ is known in Eq. (3), then it can be represented as the sum of the two following elasticity problems.

$$\begin{cases} div\sigma^E(x,t) = 0 \; \forall x \in \Omega \\ \sigma^E(x,t) = C(x){:}\varepsilon^E(x,t) \; \forall x \in \Omega \\ \langle \varepsilon^E(x,t) \rangle = \bar{\varepsilon}(t) \\ PBC \end{cases} \tag{4}$$

$$\begin{cases} div\sigma^r(x,t) = 0 \; \forall x \in \Omega \\ \sigma^r(x,t) = C(x){:}\left(\varepsilon^r(x,t) - \varepsilon^p(x,t)\right) \forall x \in \Omega \\ \langle \varepsilon^r(x,t) \rangle = 0 \\ PBC \end{cases} \tag{5}$$

Boundary value problem (4) is an equation on the RVE undergoing a certain macroscale strain as an external force when assuming that each phase of composite subjects to only elastic strain, while Eq. (5) is an equation on the RVE where a plastic strain field $\varepsilon^p(x,\mathrm{t})$, an external force, is zero and a plastic strain field $\varepsilon^p(x,t)$ acts as an eigen-strain.

From the solutions of the two elasticity problems, the solution of basic equation (3) is as:

$$\begin{cases} \sigma(x,t) = \sigma^E(x,t) + \sigma^r(x,t) \\ \varepsilon(x,t) = \varepsilon^E(x,t) + \varepsilon^r(x,t) \end{cases} \tag{6}$$

2.1. Reduced Order Model Using Proper Orthogonal Decomposition (POD)

Let a macroscale strain space be E. And let a possible plastic strain field space satisfying problem (1) be E^p. Suppose the set of sample solutions of plastic strain field, $\tilde{E}^p = \{\varepsilon_1^P(x), \varepsilon_2^P(x), \ldots \varepsilon_N^P(x)\} \subset E^p$ is created by solving directly problem (1) corresponding to the macroscale strain load path, $\tilde{E} = \{\bar{\varepsilon}_1, \bar{\varepsilon}_2, \ldots \bar{\varepsilon}_{N_1}\} \subset E$. Then, we can obtain approximation of the arbitrary plastic strain field $\varepsilon^p \in E^p$ using sample solutions as they reflect the evolutionary characteristics of E^p.

To extract the principle components from the sample solutions, the proper orthogonal decomposition can be used. Let us formulate the following correlation matrix $L \in R^{N\times N}$ as follows.

$$L_{ij} = \langle \varepsilon_i^P(x){:}\varepsilon_j^P(x) \rangle \; i,j \in [1,N]. \tag{7}$$

The correlation matrix obtained above is a positive symmetric matrix, so it has N eigenvalues λ^l and eigenvectors v^l. An information portion possessed by eigenvector v^l depends on the magnitude of λ^l. Thus, the main component can be composed as like in Eq. (8), using only eigenvector corresponding to $M \le N$ eigenvalues whose value is large, where the numbr of main componets, M is decided by Eq. (9):

$$\mu_k(x) = \sum_{l=1}^{N} v_k^l \varepsilon_l^P(x) \; k \in [1,M] \tag{8}$$

$$\beta\left(\sum_{l=1}^{N} \lambda^l\right) \le \left(\sum_{k=1}^{M} \lambda^k\right), \beta \approx 1 \tag{9}$$

In this paper, $\beta = 0.9999$. As principle components $\mu_k(x)$ of example solution set $\tilde{E}^p$ reflect evolutionary characteristics of the plastic strain field depending on the position, hereinafter called it a plastic strain mode. If a set $\tilde{E}$ of macroscale strain load path is reasonably taken at the macroscale strain space E, then any plastic strain field of possible plastic strain field space E^p can be approximately estimated using the plastic strain modes obtained: i.e.,

$$\forall \varepsilon^p \in E^p, \; \exists a_k \in R^M, \varepsilon^p(x,t) \approx \sum_{k=1}^{M} a_k(t)\mu_k(x) \tag{10}$$

Here, $a_k(t)$ is an undetermined constant, deciding changes of plastic strain field over time.

Substitute Eq. (10) into Eq. (5) and consider the linearity of the problem, then the solution of (5) can be approximately calculated by solving M proper strain problems:

$$\begin{cases}\sigma^r(x,t) \approx \sum_{k=1}^{M} a_k(t)\sigma_k^r(x) \\ \varepsilon^r(x,t) \approx \sum_{k=1}^{M} a_k(t)\varepsilon_k^r(x)\end{cases} \tag{11}$$

Here, $\sigma_k^r(x)$ and $\varepsilon_k^r(x)$ are residual stress and residual strain fields, respectively, being the solution of Problem (5) when $\mu_k(x)$ acts as proper strain.

On the other hand, virtual elastic stress and strain fields, $\sigma^E(x,t)$ and $\varepsilon^E(x,t)$ can be represented by stress concentration tensor $A(x)$ and strain concentration tensor $B(x)$:

$$\begin{cases}\sigma^E(x,t) = B(x):\bar{\varepsilon}(t) \\ \varepsilon^E(x,t) = A(x):\bar{\varepsilon}(t)\end{cases} \tag{12}$$

By substituting Eqs. (11) and (12) into Eq. (6), then the following reduced order model is obtained:

$$\begin{cases}\sigma(x,t) \approx B(x):\bar{\varepsilon}(t) + \sum_{k=1}^{M} a_k(t)\sigma_k^r(x) \\ \varepsilon(x,t) \approx A(x):\bar{\varepsilon}(t) + \sum_{k=1}^{M} a_k(t)\varepsilon_k^r(x)\end{cases} \tag{13}$$

Take volume-average of all the field information, $\varepsilon, \sigma, A, B, \sigma_k^r, \varepsilon_k^r$ in Eq. (13) in domain Ω, then the following equation (14) is obtained:

$$\begin{cases}\bar{\sigma}(t) \approx \bar{B}:\bar{\varepsilon}(t) + \bar{\sigma}^r a \\ \bar{\varepsilon}(t) \approx \bar{A}(x):\bar{\varepsilon}(t) + \bar{\varepsilon}^r a\end{cases} \tag{14}$$

Consequently, the solution of the basic equation (3) can be approximated to the solution of the reduced order model (14) which has $a = \{a_1(t), a_2(t), \ldots, a_M(t)\}$ as its unknown variable.

2.2. Numerical Solution of Reduced Order Model by Clusterization

$A(x)$, $B(x)$, $\sigma_k^r(x)$ and $\varepsilon_k^r(x)$ in reduced order model (13) are the quantities independent of external $\bar{\varepsilon}(t)$ acting on RVE and these can be decided by finite element analyses in finite times. In this time, it is very important to choose the reasonable set $\tilde{E}$ of macro strain load path in order to improve the accuracy of reduced order model. In CNTFA, macro strains distributing uniformly on a hyper-sphere with radius r_ε are taken as a trial series [16]. Also, it is assumed that the strain loads are acted monotonically.

Next, perform a region splitting by clustering to decide the coefficient $a_k(t)$ of plastic strain mode. As a result of clustering all the points (integral points) of Ω into n_c subregions (clusers) where $A(x)$ and $\mu_k(x)$, $\varepsilon_k^r(x)$ are similar to each other by using Frobenius norm, it can be seen that stress and strain within the same cluster are followed by the same physical law. Note that each cluster can be only on one phase and the clusterization must be performed at the points within the same phase. After that, the entire domain Ω can be considered to be composed of n_c integral points, so both unknown variable $a_k(t)$ and macrostress $\overline{\sigma}(t)$ can be incrementally decided using the radial-return mapping algorithm by using the constitutive equations of each phase. Denote the number of loading steps as ε_{inc} when using this algorithm.

After deciding the $a_k(t)$, we can determine the microscopic information in RVE such as $\sigma(x,t)$ and $\varepsilon(x,t)$ approximated with the results by using direct numerical simulation (DNS).

3. Data-driven Multiscale Computational Framework Using CNTFA

In the above homogenization stage to RVE, although the reduced order model CNTFA is an effective method to compute the strain-stress response in comparison with DNS, it is not so rapid to compute the response of structural level by using this. Additionally, it is impossible to compute the material effective stiffness analytically. These two disadvantages can be easily overcome by using the NN-based material constitutive modeling. Here, we can use the software such as MATLAB and PYTHON because they have built-in special purpose modules (packages) for ANN techniques.

3.1. Creating Database $D:\bar{\varepsilon} - a\bar{\varepsilon}$ Using CNTFA

In general, the accuracy of learning depends on not only the magnitude of ANN, but also the quality and quantity of learning data. If the learning data is insufficient, then the result of ANN learning is not ensured. Obtaining the experimental data by performing the experiment such as tensile test can be as a method to prepare the learning data with less errors, but it is time-consumed. A real way to prepare the material database is to use the reduced order model.

In the early studies of NN-based material constitutive models, the database consisting of paired strain $\bar{\varepsilon}$ and stress $\bar{\sigma}$ is used as learning data [6, 8]. Also, the aims of these studies were restricted to calculating the material stiffness using ANN and estimating the response of structure by using this.

However, while performing the studies to apply NN-based constitutive models to multiscale computation, a necessity to regenerate the microscale field information together with structural computation has been raised. For example, in ref. [19], after predicting the effective response, authors regenerated the cluster-wise field information to consider the microstructure damage by using convolutional neural network in the topology optimization problem. This study shows that the ability to regenerate the microscale field information is very important in solving the realistic problems such as topology optimization of periodicity composites by using data-driven multiscale analysis.

In this paper, we create a material database consisted of strain $\bar{\varepsilon}$ and the vector a using reduced order modeling CNTFA with high regeneration ability of microscale field information and estimate all of effective response, material

stiffness and microscale field information using only a feed-forward network.

First, let's analyze the characteristics of vector a in Eq. (14) to improve the quality of learning data. If a is null vector, then it means that all the points x in RVE subjected macroscale strain $\bar{\varepsilon}$ behave elastically. That is, a macroscale point $\bar{x}$ corresponding to a representative volume element at the microscale behaves elastically. On the other hand, if a is not null vector, then $\bar{x}$ behaves plastically.

This physical characteristics of a must be fully considered in preparing learning data. If the material data with null vector a is relatively larger than the other data in database, then the neural network trained in this database reflects elastic state significantly, and vice versa. As a result, a trend to over- or under-estimate the effective response appears. Thus, learning data reflecting elastic or plastic state must be appropriately involved in database. According to our computational experience, a reasonable proportion of elasticity-reflected learning data in the whole material database is 10%~15%. To satisfy this requirement in the learning data, a method for generating the learning data is proposed: First, generate a set $\tilde{E}$ consisting of N_2 macroscale strains, randomly distributing each component of macroscale strain on interval $(-1\%, +1\%)$. Next, multiply each generated macroscale strain by the following parameter α calculated:

$$\alpha(\bar{\varepsilon}) = \frac{s\sigma_y}{\bar{\sigma}_{\mathrm{eq}}(\bar{\varepsilon})} \tag{15}$$

Here, $\bar{\sigma}_{\mathrm{eq}}$ is an effetive stress corresponding to macroscale strain $\bar{\varepsilon}$ in elastic-plastic materials, σ_y is a yield stress and s is a constant related to material characteristics, playing a role to adjust the proportion between elastic and plastic states (Figure 1).

Next, denote load step number as N_{inc}, calculate a set of plastic strain mode vectors, $\tilde{A} = \{a_1, a_2, \ldots, a_{N_2}\}$ corresponding to the multiplied macroscale strains, using the reduced order model CNTFA and create a material database, $D_a: \tilde{E} - \tilde{A}$ involving total $N_T \times N_{inc}$ material behaviors.

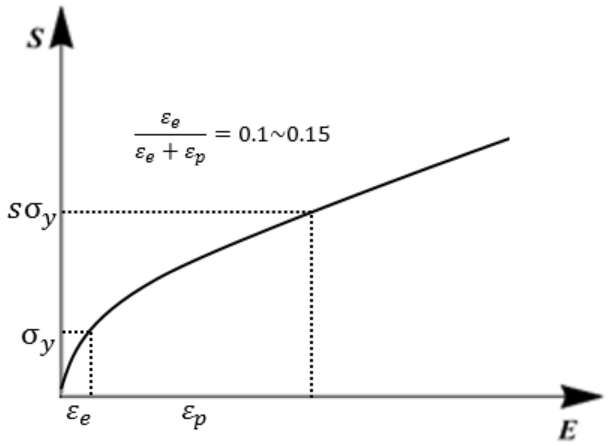


Figure 1. *Meaning of s in the stress-strain diagram.*

3.2. Feed-forward Neural Network (FFNN) for Learning the Material Behavior

ANN, a simple type of machine learning algorithm, is mainly used in nonlinear regression and classification problem. Feed-forward neural network, a neural network developed initially, consists of an input layer, several hidden layers and an output layer. The weight matrix W^h, bias vector b^h and activation function (or transfer function) f^h are the main parameters of FFNN. In the hidden layers, sigmoid (log-sigmoid, hyperbolic tangent) functions, as an activation function, are usually used, while, in output layer, identity function or soft max function is used depending on the purpose of FFNN.

The structure of FFNN is shown in Figure 2, where the number of neurons of the input and output layers are nsk and M, respectively, and $h = 3$. Set the number of neurons of hidden layer as 20. In this study, we use hyperbolic tangent function as the activation function of hidden layer, identity function as the activation function of output layer: i.e.,

$$f^h(x) = \begin{cases} \frac{2}{1+e^{-2x}} - 1 & h = 1, 2 \\ x & h = 3 \end{cases} \tag{16}$$

Then, the $FFNN_a$ outputs a^{FFNN} in the output layer for the value $\bar{\varepsilon}$ in the input layer:

$$a^{FFNN} = f^h\left(W^h\left(f^{h-1}\left(W^{h-1}\left(f^{h-2}(W^{h-2}\bar{\varepsilon} + b^{h-2})\right) + b^{h-1}\right)\right) + b^h\right) \tag{17}$$

When learning this $FFNN_a$ on a material database $D_a: \tilde{E} - \tilde{A}$, we can decide the weight matrix W^h and bias vector b^h that an error function $MSE = \sum_{i=1}^{T} \|a_i - a_i^{FFNN}\|$ becomes minimize.

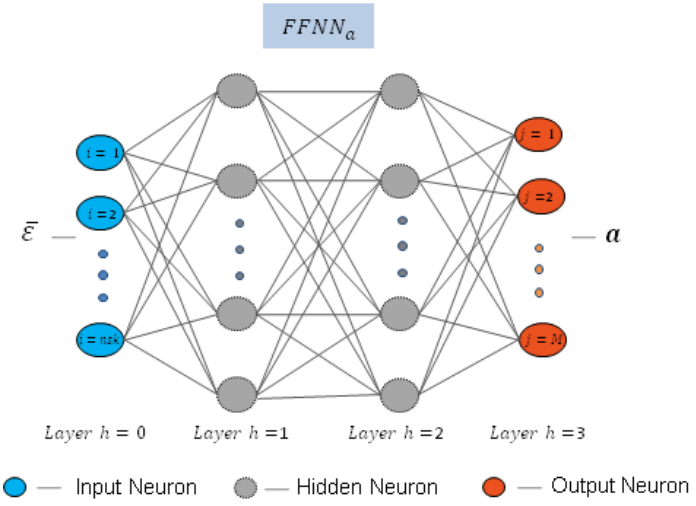


Figure 2. *Structure of* $FFNN_a$.

Substituting Eq. (17) into Eq. (14), we can calculate macroscale stress $\bar{\sigma}$ corresponding to the macroscale strain $\bar{\varepsilon}$ and substituting Eq. (17) into Eq. (13), a microscale field information.

Now, a problem to be solved is to estimate a material stiffness when subjecting a macroscale strain $\bar{\varepsilon}$. This problem can be easily solved by using the characteristics of the vector a in CNTFA. By differentiating Eq. (14) with macroscale strain $\bar{\varepsilon}(t)$, then we have

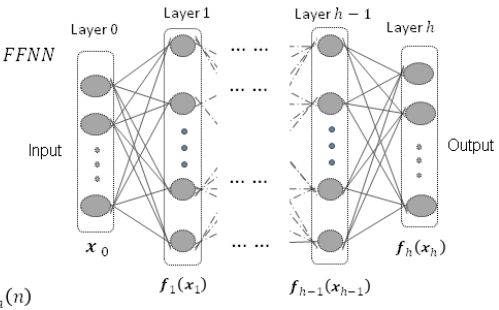
$$\frac{\partial \bar{\sigma}}{\partial \bar{\varepsilon}} \approx \bar{B} + \bar{\sigma}^r \frac{\partial a}{\partial \bar{\varepsilon}}. \tag{18}$$

Here, $\frac{\partial a}{\partial \bar{\varepsilon}}$ is a gradient of $FFNN_a$, remained terms, $\bar{B}, \bar{\sigma}^r$ are the decided in Subsection 2.1. Thus, from Eq. (18), a material stiffness of homogenized RVE can be approximately calculated by the gradient of $FFNN_a$. In refs. [8, 22], authors presented the several analytical expressions that calculate the gradient using ANN parameters, W^h, b^h. In this paper, we introduce a detailed algorithm to decide the gradient in several numerical programs on the basis of these analytical expressions (Figure 3):

After Training of FFNN

$\boldsymbol{W}_i, \boldsymbol{b}_i$: *weight matrix, bias vector in* $i-th$ *layer*
$N(i)$: *the number of neurons in* $i-th$ *layer*
$\boldsymbol{x}_i$: *input vector befor applying transfer function* f_i *in* $i-th$ *layer*
$\boldsymbol{r}_{in}$: *range vector of input learning data*
$\boldsymbol{r}_{out}$: *range vector of output learning data*

START
$i = 1$
$\boldsymbol{G} = eye(N(i))$: *indicating the gradient of FFNN*
while $(i \neq h)$
$i++$
$\boldsymbol{x}_i = \boldsymbol{W}_i \times tansig(\boldsymbol{x}_{i-1}) + \boldsymbol{b}_i$
$\boldsymbol{D} = zeros(N(i), N(i-1))$
For $j = 1, N(i)$
$\boldsymbol{D}(j,:) = \boldsymbol{W}_i(j,:)/cosh^2(x_i^j)$
end
$\boldsymbol{G} = \boldsymbol{D} \times \boldsymbol{G}$
$\boldsymbol{G} = \boldsymbol{W}_h \times \boldsymbol{G}$
$\forall m, n, \quad \boldsymbol{G}(m,n) = \boldsymbol{G}(m,n) \times \boldsymbol{r}_{out}(m) \div \boldsymbol{r}_{in}(n)$
END



*A range vector, as a normalization parameter of learning data, is calculated as a difference maximum vector and minimum vector.
A maximum(minimum) vector consists of element-wise maximum(minimum) values of all vectors in learning data.

Figure 3. *Algorithm for computing the gradient of ANN.*

3.3. Data-driven Multiscale Analysis Using CNTFA: NN-CNTFA

A boundary value problem at the macroscale can be expressed by.

$$\begin{cases} div\bar{\sigma}(\bar{x},t) = 0 \ \forall \bar{x} \in \Phi \\ \bar{\sigma}(\bar{x},t) = \bar{C}(x) : \bar{\varepsilon}(\bar{x},t) \ \forall \bar{x} \in \Phi \cdot \\ BC \end{cases} \tag{19}$$

Here, $\bar{C}(x)$ is a material stiffness $\frac{\partial \bar{\sigma}}{\partial \bar{\varepsilon}}$ calculated by the method in Subsection 3.2, Φ means an area occupied by the structure. To solve the problem (19) in the finite element analysis software ABAQUS, we develop a material user subroutine UMAT. Then, store a_k computed at each integral point at the macroscale using SDVs in UMAT. Also, read the SDVs stored at each integral point and develop the ABAQUS Python script to regenerate the microscale field information from Eq. (13). Figure 4 shows a framework of data-driven multiscale analysis NN-CNTFA following the computational process in Section 2 and 3.

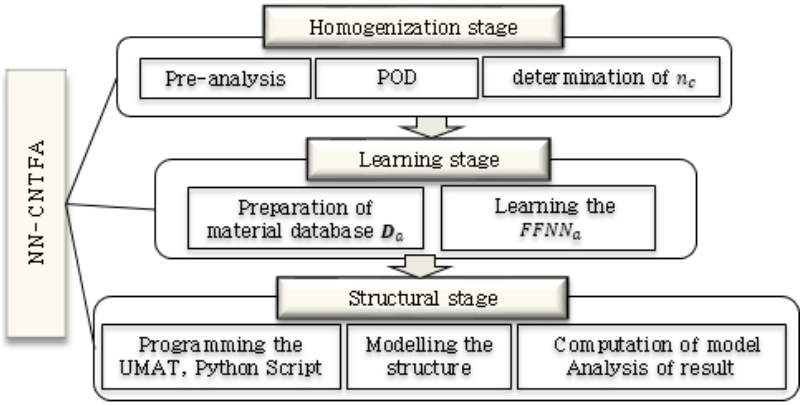


Figure 4. *Framework of data-driven multiscale analysis NN-CNTFA.*

4. Verification of NN-CNTFA

All the computations have been carried out by using the computer with 8GB RAM of Intel® Core (TM) i7-4790CPU@3.60GHz, finite element analysis software ABAQUS 6.14-1 and MATLAB 2018a.

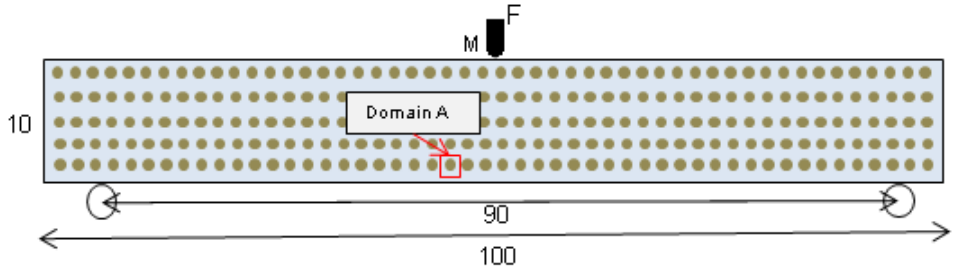


Figure 5. *Rectangular beam under three-point bending.*

Consider a three-point bending problem of boron-aluminum composite beam shown in Figure 5 as an example problem. Assume that the length unit in all figures is mm. As shown in Figure 5, the beam made of composite in which the volume ratio of boron inclusion is 30% is periodically arranged. That is to say, the model of Figure 6 can be considered as RVE. Taking into account the geometry and boundary condition of a beam subjected three-point bending, this problem can be reduced to an axisymmetric plane strain problem. Young's modulus and Poisson ratio of aluminum material as the matrix of composite are $E_1 = 75\text{GPa}$, $\nu_1 = 0.3$, respectively. For a material model, the following isotropic hardening rule is used:

$$f = \sigma_{eq} - \sigma_{y0} - hp^m = 0 \tag{20}$$

Here, $\sigma_{y0} = 75MPa$, $h = 416.5MPa$, $m = 0.3895$, and p is an effective plastic strain. Young's modulus and Pois-

son ratio of boron material as the inclusion of composite are $E_2 = 400GPa,\ \nu_2 = 0.2$.

In the homogenization stage, establish a reduced order model CNTFA for RVE in Figure 6. For meshing of RVE, 1,888 linear quadrilateral sequential elements are used.

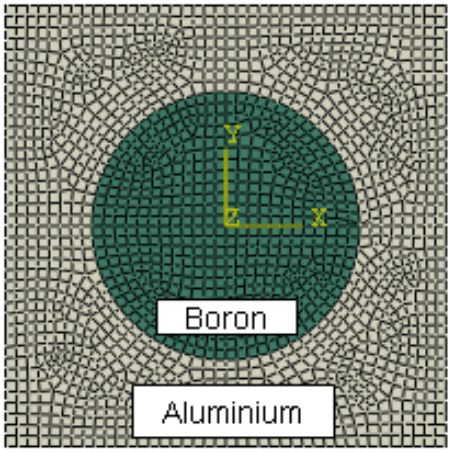


Figure 6. *Mesh of RVE.*

As a result of proper orthogonal decomposing using 8 learning load paths distributed uniformly on a sphere with radius of 0.05, $M = 15$ plastic strain modes are obtained. Consequently, the vector a and effective response $\bar{\sigma}$ of (14) can be effectively calculated after the elements of RVE are divided into several clusters by the method described in Subsection 2.2. Now, although the more the number of clusters, the better the accuracy of reduced order model CNTFA, the effectiveness conversely becomes worse due to increasing computational time. Further, it will take more times to prepare a material database involving a lot of material behaviors. So, the number of clusters n_c must be decided to balace between accuracy and effectiveness of CNTFA: in this paper, we set $n_c = 25$. The time consumed for establishing a reduced order model CNTFA is 331.1s, while the response time of CNTFA when subjected by strain load is 12.8s.

In learning stage, set $N_{inc} = 100$, $N_T = 1{,}200$ and prepare a material database involving total 120,000 paired data using the reduced order model CNTFA. After finished this preparation, perform the learning $FFNN_a$ as like in Subsection 3.2 and output the data file in which the parameters of $FFNN_a$ such as weight and bias values are included. Using this file, make a material user subroutine UMAT to compute effective stress and material stiffness. In this UMAT, a_k are stored in $M = 15$ SDVs, allowing to regenerate microscale field quantities as like in (13). It takes approximately 51,360s for generating the material database and learning of $FFNN_a$, and the response time of it is 0.27s. Before the structural stage, let us consider the accuracy and effectiveness of NN-CNTFA in comparison with DNS and CNTFA. Figure 7 shows Mises stress estimated comparatively using DNS, CNTFA and NN-CNTFA for a strain load, $\bar{\varepsilon} = 0.005 \times (1, -0.3, 0, 1)$. From this figure, the effective Mises stress estimated by using CNTFA and NN-CNTFA coincides with the result of DNS with errors of 1.2% and 1.8%, respectively. On the other hand, CNTFA and NN-CNTFA are respectively quicker 2 and 60 times in compared with DNS (the more the number of elements in RVE, the higher the computational effectiveness of CNTFA and NN-CNTFA).

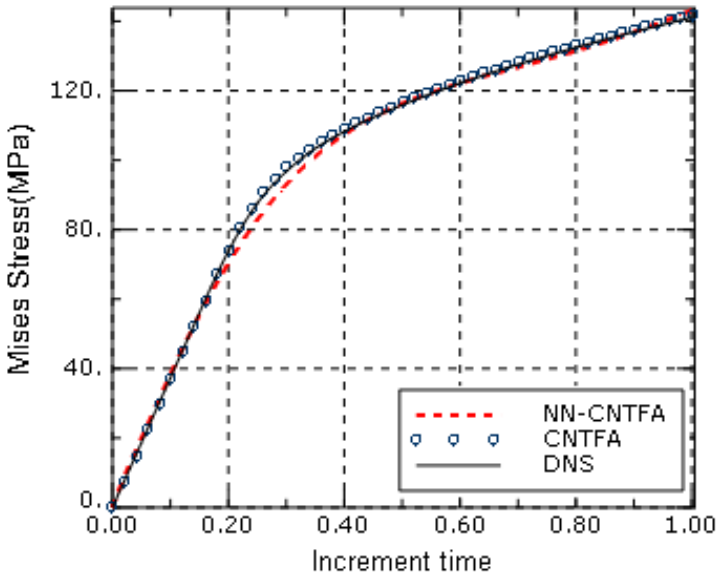


Figure 7. *Comparison of Mises stress estimated by using CNTFA, NN-CNTFA and DNS.*

In the last structural stage, let us analyze a bending problem of beam assumed as homogeneous materials using UMAT. Both of the supporting point and the pressing point are modeled as an analytic rigid body with radius of 2, all the degrees of freedom is fixed and the beam are loaded by displacement load $U = 0.6$. Then, when loading, apply the interactions with no tangent friction between supporting point and lower surface of beam, pressing point and the upper surface of beam. The model of structure is meshed with 125 CPE4 ($2 \times 2\ mm$) elements. That is, the order of freedom of the model can be reduced down to $1/1{,}888$ by the homogenization. Figure 8 shows a bending deformation state of a beam simulated using NN-CNTFA, comparing with the result of DNS. As shown in this figure, we can see that the contours of the field information of Mises stress are similar with each other, but that there is a few difference in the magnitude.

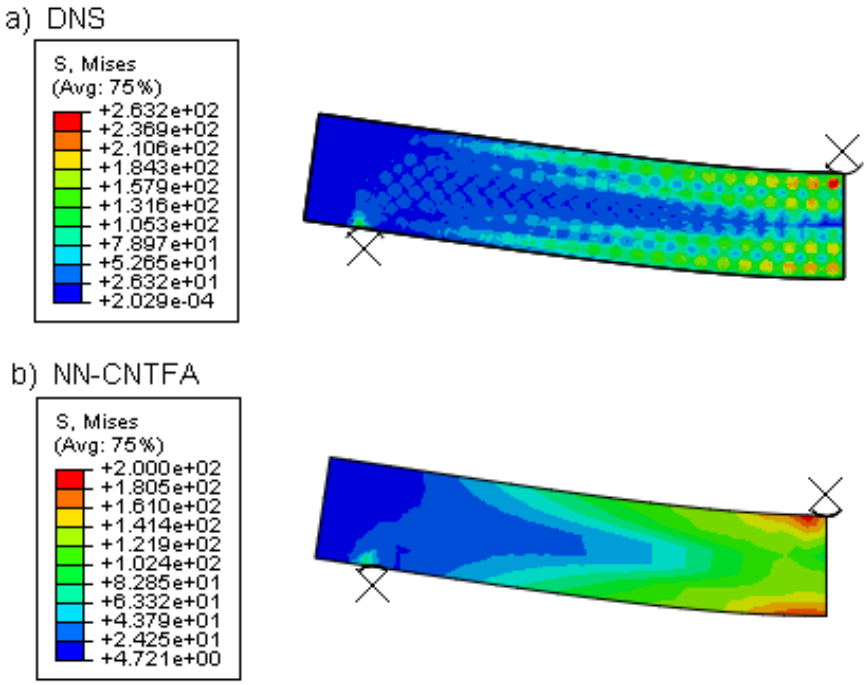


Figure 8. *Deformation state of beam subjected bending: a) DNS, b) NN-CNTFA.*

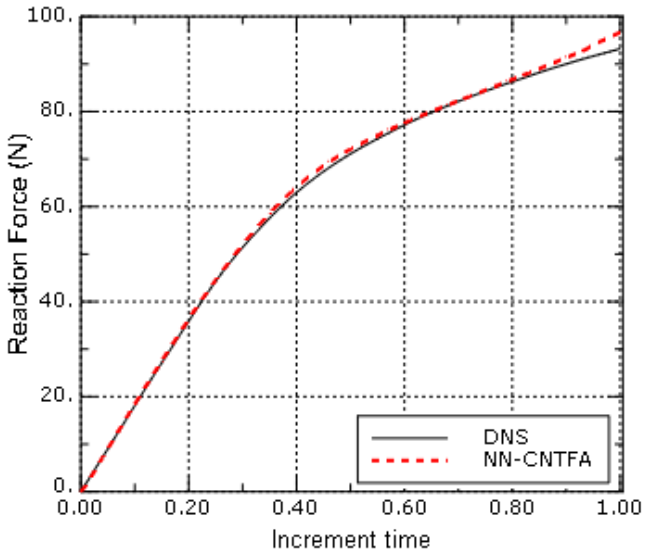


Figure 9. *Reaction force at the point M simulated by using DNS and NN-CNTFA at the macroscale.*

Figure 9 shows a reaction force at the point M placed on the center of beam. As shown in the figure, the result curves simulated by using NN-CNTFA and DNS are very approximated with the error of 3.2%. Meanwhile, it takes 16.6s for computation by using NN-CNTFA, suggesting that the computational efficiency of NN-CNTFA is higher about 351 times in compared with 5,829s consumed when DNS is used.

Figure 10 shows the distributions of microscale stress simulated by using DNS and NN-CNTFA in RVE corresponding to domain A. It can be seen that there is a few difference in the distribution characteristics of Mises stress, but that its maximum and minimum values are similar each other. If the mesh becomes denser at the macroscale, then this difference will be gradually reduced.

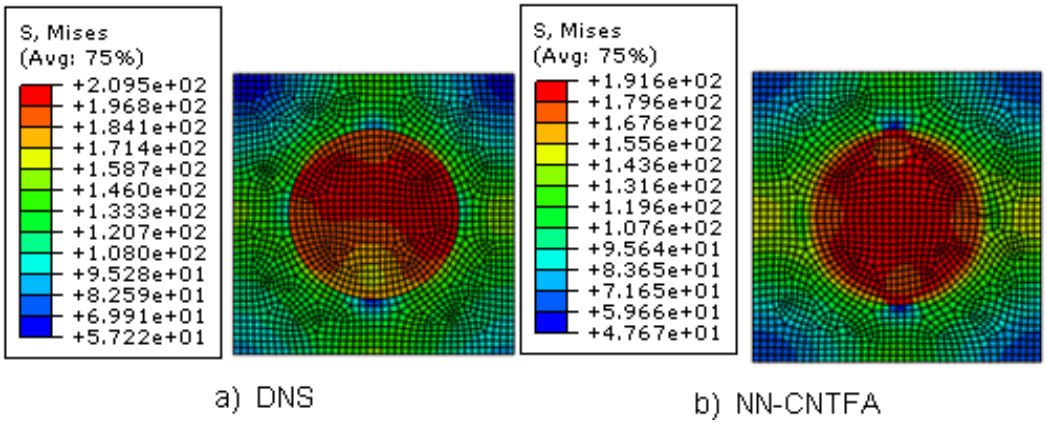


Figure 10. *Distribution of Mises stress simulated by using DNS and NN-CNTFA in Domain A.*

5. Conclusion

In this paper, a data-driven multiscale analysis NN-CNTFA have been proposed by using ANN and CNTFA. In this computational framework, the material constitutive model can be considered as the gradient of ANN learned on the material database which is generated by using CNTFA and it is complemented with the material user subroutine UMAT. Thus, this computational method can be used in the computing tools such as ABAQUS and ANSYS with built-in FEM, so that the post processes such as strain state visualization and data output are available. The important characteristics of NN-CNTFA distinct from other cluster-based data-driven computational method is to regenerate the microscale field information at material (integral) point. The accuracy and effectiveness of the presented method have been proved through the computational example of 2D problem of three-point bending. In this example, detailed procedures to run NN-CNTFA have been fully described. In comparison with the DNS, it has been proved that NN-CNTFA is an effective method by which a nonlinear analysis of composite structure can be performed at high accuracy.

Abbreviations

ANN	Artificial Neural Network
CNTFA	Cluster-based Non-uniform Transformation Field Analysis
DNS	Direct Numerical Simulation
FCA	FEM Clustering Analysis
FFNN	Feed-forward Neural Network
MSE	Mean Squared Error
NN-CNTFA	Neural Network Cluster-based Non-uniform Transformation Field Analysis
NTFA	Non-uniform Transformation Field Analysis
POD	Proper Orthogonal Decomposition
RNEXP	Radial Numerically Explicit Potentials
RVE	Representative Volume Element
SCA	Self-consistent Clustering Analysis
TFA	Transformation Field Analysis
VCA	Virtual Clustering Analysis

Conflicts of Interest

The authors declare no conflicts of interest.

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