Machine learning-assisted two-step homogenization framework of short fiber-reinforced plastics

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ABSTRACT

Short fiber-reinforced plastics (SFRPs) are extensively utilized in the automotive and aerospace fields due to their superior ease of manufacturing, affordability, and exceptional mechanical properties. However, as automotive components made from SFRPs encounter intricate mechanical stresses, it is necessary to have an accurate micro-mechanical model for their mechanical behavior prediction. In this study, we propose a machine learning-assisted two-step homogenization framework of short fiber-reinforced plastics (SFRPs). A series–parallel artificial neural network (ANN) system is constructed and trained to facilitate the time-consuming reconstruction of orientation distribution function and pseudograin decomposition procedures. Then, we incorporated the series-parallel ANN system, Mori-Tanaka model, and Voigt model into ABAQUS user material subroutine (UMAT). The elastic moduli predicted by UMAT were in good agreement with experimental values, thereby showing the validity of the proposed framework.

1 INTRODUCTION

The demand for short fiber-reinforced plastics (SFRPs) is on the rise in the automotive and aerospace industries, primarily due to their cost-effectiveness, superior mechanical properties, and design flexibility [1]. However, since SFRP automotive parts experience intricate loading, it's crucial to have the ability to predict their complex behavior. Therefore, a fundamental approach that can simulate the mechanical response of SFRPs is needed. The most comprehensive method used for mechanical behavior prediction of SFRPs considers mean-field homogenization methods based on Eshelby's single inclusion theory [5], such as the Mori– Tanaka model [6], self-consistent model [7], double-inclusion model [8], and differential scheme model [9]. However, these homogenization models are unsuitable for interpreting SFRPs because these models require the target composite to have inclusions of similar shape and orientation [10]. Various studies have explored the pseudograin approach as a two-step homogenization procedure, which was first suggested by Pierard et al. [10] to overcome the constraints of direct finite element simulation. This technique involves assumption that the short fibers in each pseudograin are elastic and aligned in a single direction, with a representative orientation derived from processing the orientation distribution function (ODF). For ODF reconstruction method, Maximum Entropy (ME) method is one of the popular choices examining the fiber orientation of all positions, specifically for injection molded SFRPs. However, determining the optimum parameters of Bingham distribution for ODF reconstruction and pseudograin decomposition procedures of SFRP parts require massive computational cost, especially when it comes to iterative minimization procedure. To address this problem, we examined research that utilized artificial neural networks (ANNs) to decrease computational expenses in the field of constitutive modeling of composite materials. In this study, we proposed a machine learning-assisted two-step homogenization framework for short fiber-reinforced plastics (SFRPs). A series-parallel artificial neural network (ANN) system was constructed and trained to facilitate the reconstruction of time-consuming orientation distribution function (ODF) and thus to enable to repudiate pseudograin decomposition procedures. Then, we implemented the series-parallel ANN system, Mori-Tanaka model, and Voigt model to ABAQUS user material subroutine (UMAT). The elastic modulus values predicted by UMAT were in good agreement with both DIGIMAT and experimental values, maintaining low computational time. The graphical abstract of the overall procedure of our study is provided in Figure 1.

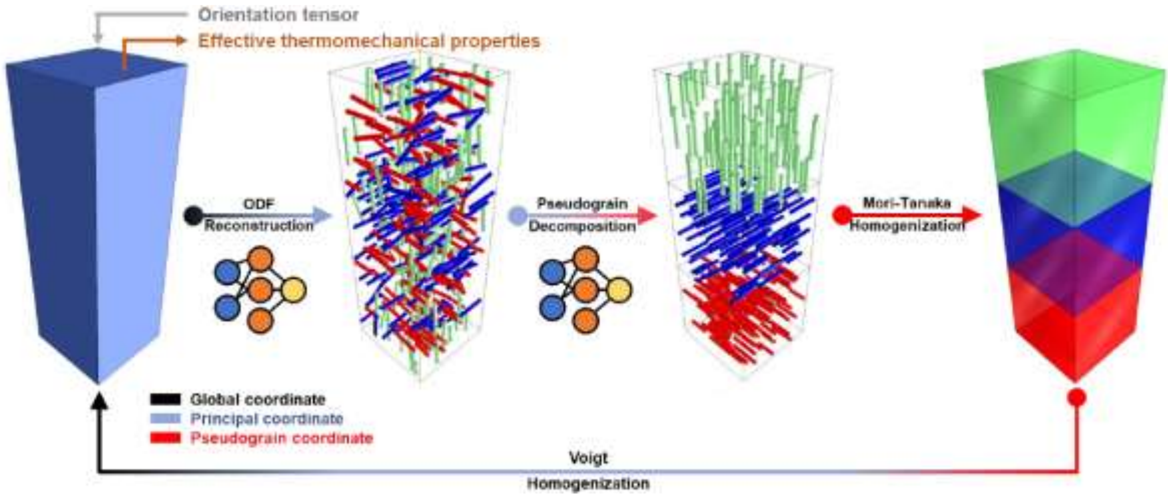

Figure 1: Schematic diagram of the overall procedure; the color change of the arrow indicates the rotation of the coordinates

2 THEORETICAL BACKGROUND

2.1 Reconstruction of fiber orientation distribution function (ODF)

Utilizing the orientation tensor for the mechanical simulation of SFRPs poses a significant challenge because two distinct ODFs can have identical orientation tensors. Thus, there is a need for a reconstruction model that can identify a specific ODF when a particular orientation tensor is provided. The most widely used model is the Maximum Entropy (ME) reconstruction model [11], which is based on empirical observation that the microstructures of injection molded SFRPs tend to have maximum entropy. The presented research discovered that the ODF with the maximum entropy can be expressed as equation (1), which involves a bivariate Bingham distribution on the unit sphere. The parameters of this distribution are α and β. Under this given situation, entropy (S) and orientation tensor (a_{ij}) can be described as equation (2) and (3). In last, the minimization procedure of Pareto optimization method was adopted to determine the α and β values that would optimize the entropy value in the final step of the ODF reconstruction procedure.

$$\psi(\mathbb{P}_k) = Ce^{-\alpha P_{3k}^2 + \beta P_{1k}^2} \ . \tag{1}$$

$$S = -\sum_k \psi(\mathbb{P}_k) \ln(\psi(\mathbb{P}_k)) \ . \tag{2}$$

$$a_{ij} = \sum_k P_{ik} P_{jk} \psi(\mathbb{P}_k) \ . \tag{3}$$

2.3 Pseudograin decomposition

Once the reconstruction process is finished, the ODF is disintegrated into multiple pseudograins that contain short fibers aligned in a single direction. The decomposition process is designed to meet the homogenization models' criteria, which mandate that composites should have inclusions with comparable orientation and shape. In this current study, we opted to use a weighted k-means clustering algorithm instead of evolutionary algorithm to significantly decrease computational time while preserving a high level of precision. K-means clustering algorithm, also known as Lloyd's algorithm [12], is an algorithm used to divide a set of n data points $\mathbb{X} = (x_1, x_2, \ldots, x_n)$ into k ($\leq n$) clusters. The algorithm begins with defining a set of k arbitrary centroids $\mathbb{C} = (c_1, c_2, \ldots, c_k)$ that is selected uniformly and randomly from $\mathbb{X}$. Each data point in $\mathbb{X}$ is then assigned to the nearest centroid based on Euclidean distance, and the data points assigned to the same centroid form a cluster. Consequently, the Centroid $\mathbb{C}$ is updated by finding the center of mass of the data points in the same cluster. The process is repeated until the change in centroid position becomes smaller than the tolerance value. Different from general k-means clustering, weighted k-means clustering assigns weights $\mathbb{W} = (w_1, w_2, \ldots, w_n)$ to each data point $\mathbb{X}$ when calculating the new center of mass $\mathbb{C}$.

3 MATLAB IMPLEMENTATION

3.1 MATLAB implementation of ODF reconstruction and pseudograin decomposition procedure

The process of reconstructing the ODF and decomposing pseudograins was carried out using MATLAB. The icosphere algorithm was used to divide a unit sphere into triangular meshes. As previously mentioned, Pareto optimization was utilized to find two parameters of bivariate Bingham distribution that maximizes entropy. Additionally, Additionally, the weighted k-means clustering was initialized using the k-means++ seeding algorithm. Note that the number of clusters, denoted as pseduograins in this concept, were fixed to 12 for overall convenience.

4 APPLICATION OF MACHINE LEARNING APPROACH

4.1 Series-parallel ANN system

A series–parallel ANN system consisting of five fully connected ANNs was proposed to train ODF reconstruction and pseudograin decomposition procedures. The initial ANN in the series-parallel architecture is labeled as "OT2AB". This name indicates that it takes diagonal orientation tensor (OT) data as input and produces the α and β (AB) parameters of the bivariate Bingham distribution as output. The 2nd–4th ANNs are named after "AB2TPGi" (i=1,2,3), which imply that they provide equivalent orientations (θ, ϕ) of PG1, PG2, and PG3, respectively, from α and β input data obtained from OT2AB. To generate the remaining information for PG4 to PG12, the data from PG1-PG3 was reflected sequentially about the x-axis, y-axis, and origin.

4.2 Training series-parallel ANN system

For the purpose of training the series-parallel artificial neural network system, 10,000 diagonal orientation tensors were generated. The accumulated data produced by the proposed series-parallel ANN system was then trained using the MATLAB Deep Learning Toolbox, with the mean squared error employed as the performance metric. The acceptable training result for OT2AB is presented in Figure 3 as a regression plot and training state plot, with approximate metric R-square value of 0.99. Identical training procedures were conducted for remaining other four ANNs (AB2PG1, AB2PG2, AB2PG3, AB2VF), all of which showed successful training performance as well (Figure 4).

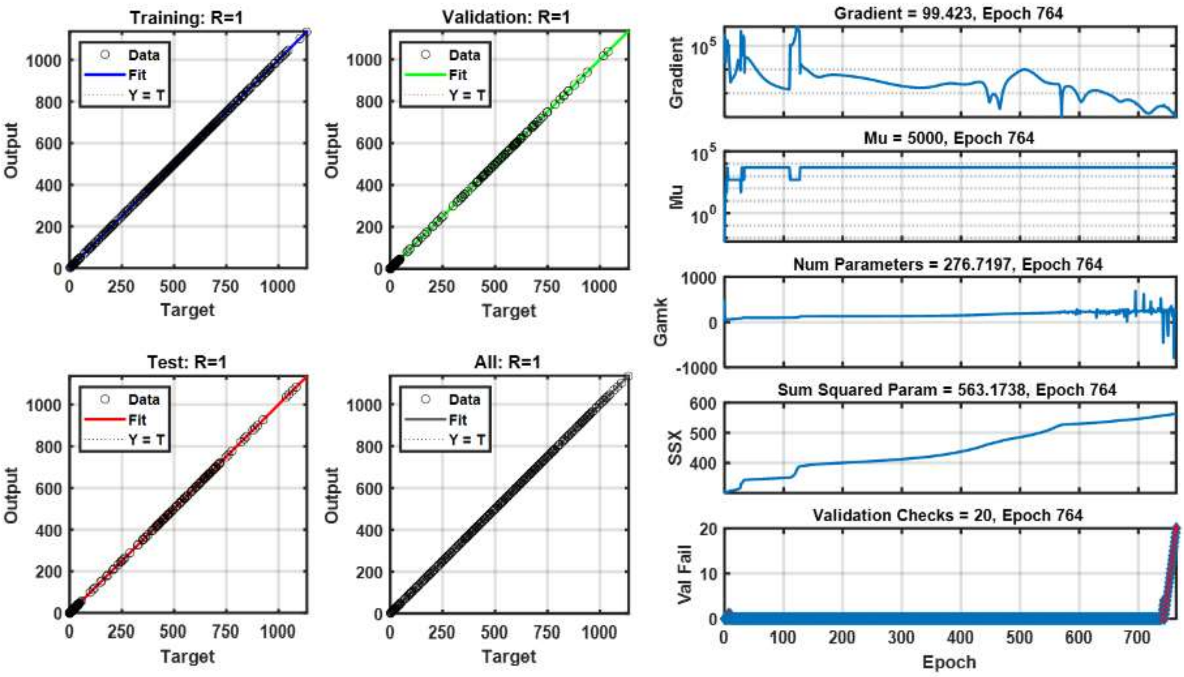

Figure 3: Regression and training state plots of OT2AB training results

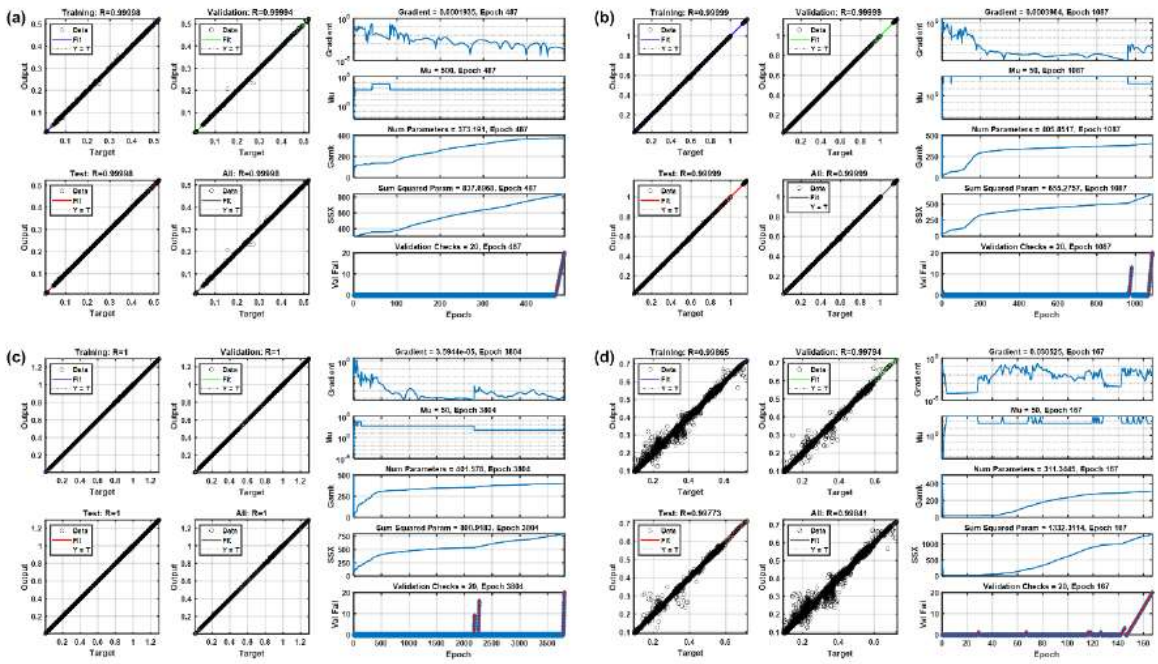

Figure 4: Regression and training state plots of (a) AB2PG1, (b) AB2PG2, (c) AB2PG3, and (d) AB2VF training results

4.3 UMAT implementation and validation

A machine learning-assisted two-step homogenization procedure consisting of series-parallel ANN system, Mori-Tanaka, and Voigt model, was implemented into ABAQUS via UMAT (see Fig. 1).

Validation of the proposed method was carried out by conducting simple tensile test simulations for two diagonal orientation tensors at opposite extremes and six non-diagonal orientation tensors. As a result, tensile behavior simulation results made by UMAT and DIGIMAT are compared in Figure 5. The results of the simulations showed that the tensile stress-strain curves obtained by UMAT had an average error of within 2% compared to DIGIMAT, regardless of the specific features of the target orientation tensor. Hence, corresponding result confirmed the validity of utilizing a series-parallel ANN system for UMAT simulation.

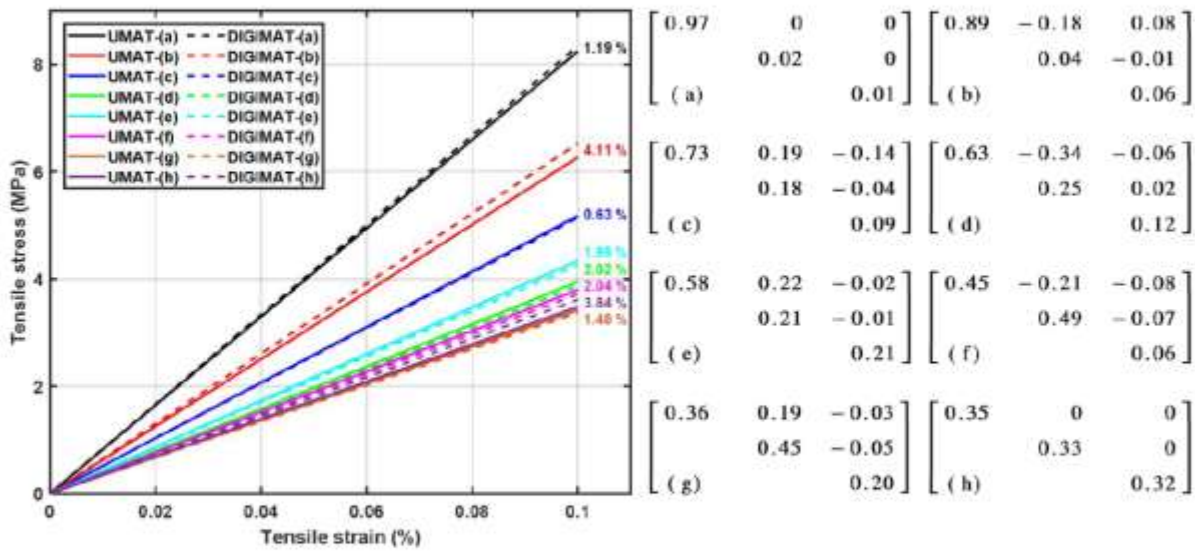

Figure 5: Comparison of tensile stress-strain curves obtained by UMAT and DIGIMAT for various orientation tensor cases

5 CONCLUSION

In this study, a machine learning-assisted two-step homogenization framework of SFRPs was proposed. ME reconstruction model and weighted k-means clustering algorithm were adopted to formulate12 pseudograins with effective orientations and volume fractions based on a given arbitrary orientation tensor. Nevertheless, due to the computationally intensive and iterative nature of both models, this methodology was not suitable for implementation in a user material subroutine of commercial finite element analysis software. To overcome this limitation, this study developed and trained a series–parallel ANN system using pre-calculated input and output data. To establish a two-step homogenization framework, the study integrated the series-parallel ANN system, Mori-Tanaka model, and Voigt model into the ABAQUS UMAT subroutine. The elastic modulus values predicted using UMAT demonstrated good performance, with less than 2% error compared to experimental values.

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REFERENCES

[1] Mortazavian, Seyyedvahid, and Ali Fatemi. "Fatigue behavior and modeling of short fiber reinforced polymer composites: A literature review." International Journal of Fatigue 70 (2015): 297-321.

[2] Sun, C. T., and R. S. Vaidya. "Composite Science and Technology." (1996): 171-179.

[3] Feyel, Frédéric. "Multiscale FE2 elastoviscoplastic analysis of composite structures." Computational Materials Science 16.1-4 (1999): 344-354.

[4] Breuer, Kevin, and Markus Stommel. "Prediction of short fiber composite properties by an artificial neural network trained on an RVE database." Fibers 9.2 (2021): 8.

[5] Eshelby, John Douglas. "The determination of the elastic field of an ellipsoidal inclusion, and related problems." Proceedings of the royal society of London. Series A. Mathematical and physical sciences 241.1226 (1957): 376-396.

[6] Mori, Tanaka, and Kohichi Tanaka. "Average stress in matrix and average elastic energy of materials with misfitting inclusions." Acta metallurgica 21.5 (1973): 571-574.

[7] Hill, Rodney. "A self-consistent mechanics of composite materials." Journal of the Mechanics and Physics of Solids 13.4 (1965): 213-222.

[8] Nemat-Nasser, Siavouche, and Muneo Hori. Micromechanics: overall properties of heterogeneous materials. Elsevier, 2013.

[9] McLaughlin, R. "A study of the differential scheme for composite materials." International Journal of Engineering Science 15.4 (1977): 237-244.

[10] Pierard, O., C. Friebel, and Issam Doghri. "Mean-field homogenization of multi-phase thermo-elastic composites: a general framework and its validation." Composites Science and Technology 64.10-11 (2004): 1587-1603.

[11] Wu, Nailong. The maximum entropy method. Vol. 32. Springer Science & Business Media, 2012.

[12] Lloyd, Stuart. "Least squares quantization in PCM." IEEE transactions on information theory 28.2 (1982): 129-137.s