EXPERIMENTALLY TRAINED PHYSIC-INFORMED NEURAL NETWORK AS MATERIAL MODEL

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Abstract:

The authors propose a new approach for the data-driven discovery of composite material models leveraging on physic informed mechanistic neural networks. The methodology is unsupervised since the surrogate neural network can learn the unexplicit constitutive law from the strain field and global force data of mechanical tests, that can be easily collected with digital image correlation technique. The approach integrates the distinctive characteristics of both mechanistic data science and physic informed neural networks: the neural network architecture is designed to predict a constitutive law respecting the material symmetry and decoupling of the axial and shear response; the data-driven model is trained with a custom loss function enforcing the equilibrium constraints between external and internal energy. The results of the training is a physic-informed neural network predicting the response of composite. Using experimental data on tensile tests of carbon fiber woven reinforced epoxy specimens, authors demonstrate the capability of the data-driven method to efficiently discover the mechanical response of composite material with a reduced set of experiments.

Keywords: mechanistic; digital image correlation (DIC); machine learning; material law; surrogate model;

1. Introduction

Experimental characterization of composite materials requires an extensive set of experiments to properly assess their mechanical properties. Especially in applications where the post-failure behavior must be experimentally investigated, the experimental campaign is expensive and the characterization and material model selection is perpetuated through trial and error loops guided by the engineer's expertise. This work propose a methodology to learn constitutive laws from Digital Image Correlation measurements by a mechanistic Physic Informed Neural Network (PINN). Recently, [1-6] has proven the capability of standard and PINN to capture the constitutive behavior of complex material systems from artificial dataset. The proposed approach is tested with experimental data of carbon fiber twill fabric reinforced epoxy subjected to tensile test.

2. Materials and experimental tests

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The composite under study is a prepreg made of GG630T-37 12K carbon fiber woven by Microtex Composites with a 2 by 2 twill fabric pattern and the E3-150N series thermosetting epoxy resin prepreg. Specimens are cut by a plate manufactured in autoclave with a maximum pressure of 6 bars and curing temperature of 125° C. Coupons have been visually inspected and no evident defect or milling induced delamination was visible.

Cross-ply specimen are made of 3 layers with 0°/90°, while angle-ply coupons have +45°/-45° orientated layers. All specimen have a total length of 250 mm, while the with is either 12, 24 or 36 mm. Plate thickness has been measured before milling in six different locations of the plate, showing an average value of 2.05 mm. For sake of brevity, the coupons will be referred as LWD_# with: L indicating if it is a cross-ply (C) or an angle-ply (A), W indicating the width (1: 12mm, 2: 24mm, 3: 36mm), D indicating the hole diameter over width ratio (0: no hole, 1: 1/12, 2: 1/6, 3: 1/4), followed by the trial number. As example, C23_2 will refer to the second trial of the cross-ply (C) lay-up test with a width of 24mm (2) and an D/W ratio of 1/4 , yielding to a 3 mm hole diameter.

Tensile tests are performed with the hydraulic powered testing machine Instron 8801, with a maximum load capability of 150 kN. Tensile tests are performed following D6390 standards, with a constant displacement rate of 2 mm / min.

Every test has been recorded with high-precision cameras and processed with Digital Image Correlation (DIC) system synchronized with the testing machine digital acquisition system.

As results of the experimental campaign, for each tensile test the following data are available:

- Crosshead displacement sampled every 0.05 seconds
- Crosshead tensile load sampled every 0.05 seconds
- Longitudinal, orthogonal and shear strain measures on the coupon surface every 0.5 second

Thanks to the synchronous measurements system, each strain map can be associated to the crosshead displacement and measured load at the instant of the acquisition (Figure 1).

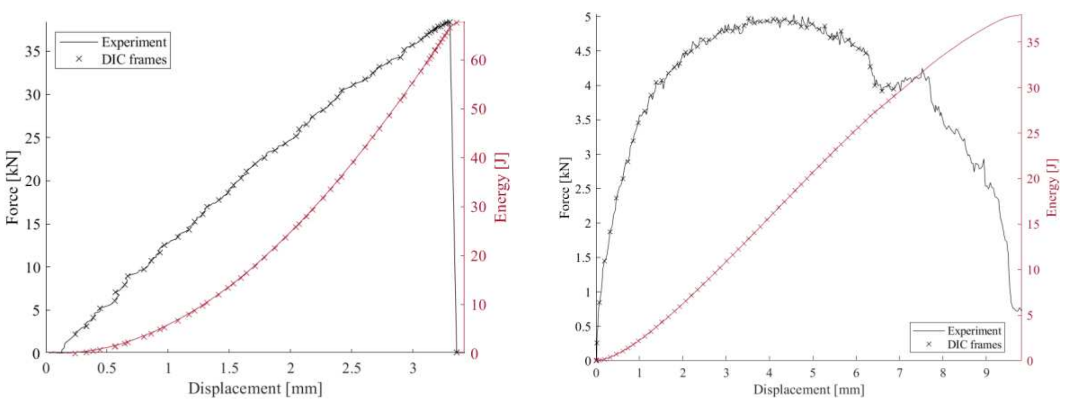

Figure 1. Force displacement curve for cross-ply (a) and angle ply (b) laminate with cross marks indicating the DIC acquisition frames

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3. Method

The simplest constitutive models are a causal relation between a measurable quantity ε , the strain, and an engineering abstraction σ, the stress. In fact, the mechanical stress is not experimentally measurable; it is a indirectly measured quantity that can be computed from the experimental tests results following calculations usually described by the standards. Training a neural network to learn a constitutive equation from experimental data is not a trivial task, since the output of the network should be first computed from the measured force, according to pre-defined equations with assumptions that inevitably introduce bias in the learning process. To overcome this issue, [7] proposed a framework for learning indirectly measurable relation and applied to it for learning the failure surface of composite from analytical data. In this work, authors want to extend the capability of the network, not only learning the failure limit, but the complete constitutive law. [8] demonstrated that a parametric constative law for hyperplastic materials can be trained on strain field and force-displacement curve of experiments and validated their work on artificially simulated experiments. The presented research, aim at training a Neural Network to learn the constitutive equation of fiber reinforced composite, by only constraining the solution with physical knowledge on composite materials, letting the machine learning structure to find the best feasible interpolation on the experimental data.

2.1 Time and space filters

When Neural Network are used to perform regression over observed data, there is the risk of overfitting the training data. Especially when dealing with experimental measures, the signal noise could worsen the performance of the minimization algorithm, yielding to an overfitting of the noisy data. In this regard, data preprocessing is a crucial step in mechanistic machine learning pipelines, where mechanistic principles could be violated by non-physical noisy observation. The strain measured with DIC during the tensile tests is affected by both space and time domain noise. These can be separately processed to remove signal information that are not descriptive of the observed phenomena. In this work, each strain component time history of each element is fitted with a cubic function as shown in Figure 2.

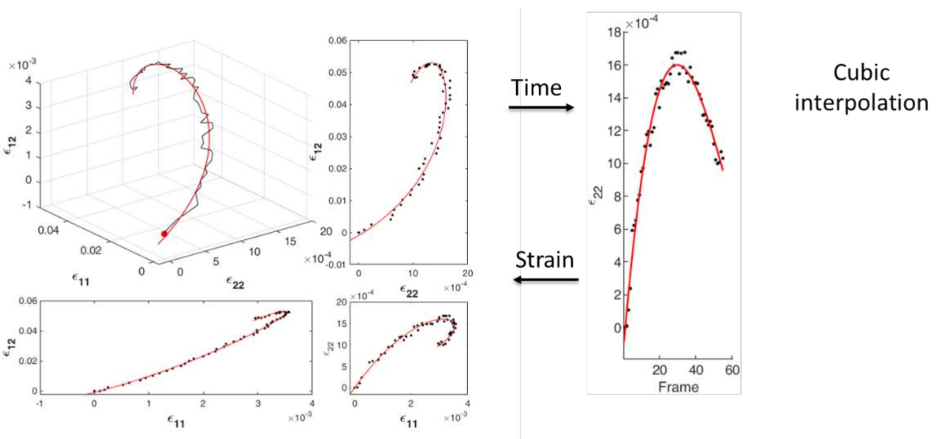

Figure 2. The three components of the strain history of each element are fitted with a cubic function of the time to remove the signal noise.

The spatial resolution of DIC depends on the camera resolution, distance from the object, subset size and other prost-processing parameters (e.g., displacement interpolation function). For the here presented experiments, the spatial resolution is approximately 0.2 mm. Since the final goal of the work is to find a surrogate material law of the homogenized material, it is mandatory to compare the resolution of the strain field with the Representative Volume Element (RVE) of the fiber reinforced material under study. Figure 3 shows the size of a Twill 2x2 RVE compared with the specimen dimension.

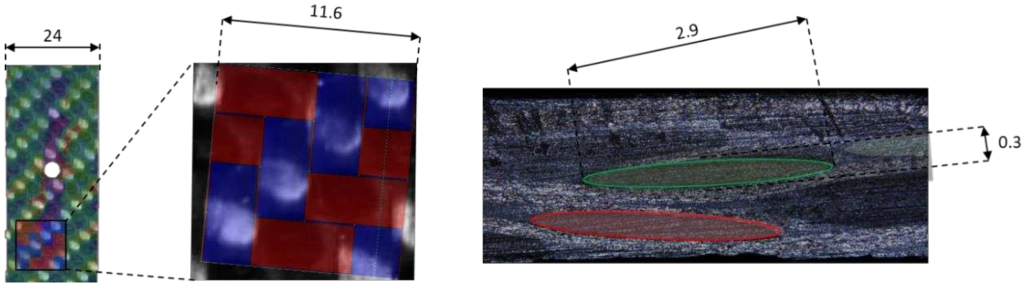

Figure 3. a) Magnification of the specimen surface with woven architecture scale length, b) cross-section of the woven specimen

Being the resolution of the DIC acquisition system lower than the RVE size, the strain is not representative of the homogenized materials. To pass the Neural Network a strain field it can learn an homogenized material law from, a spatial convolutional filter is applied to strain maps.

2.2.1 Feed-forward neural networks (FFNN)

Supervised Feed-forward neural networks (FFNN) are traditionally trained with a set of input and output observation that the network will relate through a general operator $\mathbb{N}(w_i, b_i)$, where trainable parameters w and b are the weights and biases of the network, respectively. Since the final goal of the research is to train the network on experimental data and the stress is not measurable, the network is trained to predict a local plane stress vector $\boldsymbol{\sigma_e}$ in each point of the structure from the local strain state $\boldsymbol{\varepsilon_e}$ as described in equation (1):

$$\boldsymbol{\sigma_e} = \mathbb{N}(\boldsymbol{w}, \boldsymbol{b}; \boldsymbol{\varepsilon_e}) \tag{1}$$

the total internal energy Π_i is computed at each observation i by summing the internal energy of all the N elements of the domain Ω_e using equation (2):

$$\Pi_i = \sum_{elem}^{N} \frac{1}{2} \int_{\Omega_e} \boldsymbol{\varepsilon}_e^T \boldsymbol{\sigma_e} d\Omega_e \tag{2}$$

The loss function over N_f observations, is defined by equation (3) as the root mean squared error:

$$\mathcal{L} = \sum_i^{N_f} \sqrt{\frac{\left(\Pi_i - \int_0^{d_i} f dx\right)^2}{N_f}} \tag{3}$$

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Where f is the load as function of displacement, d_i is the crosshead displacement at the observation instant i and the integral is the external work. The integral is computed using the trapezoidal rule.

The network is optimized with a stochastic gradient descent method (Kingma et al.) and the trainable parameters are upgraded with a back-propagation procedure, to minimize the loss function. Since the constitutive equation is the same for every material point, $\mathcal{N}$ is unique: to properly train it on the presented data, the number of element in each batch is set equal to the number of element in the structure and the loss function is computed at each batch.

2.2.2 Physic-informed FFNN

Neural networks have been demonstrated to be universal approximators of any functions, but the accuracy of the interpolation is strongly dependent on the amount data. For this reason, the implementation of such methods has been for a long while rarely adopted in scientific application, where dataset are usually small. In last decades, researcher has proposed a new approach for training machine learning algorithm on physic data: physic informed neural network. Several studies demonstrated that coupling the prior physical knowledge of the observed phenomena, with the approximation capability of the neural network can give good results even with small datasets. Along that line, authors propose a Physic-informed FFNN (PI-FFNN) trained on the experimental data of tensile tests coupled with the physic principles of material symmetry and energy conservation.

Starting from the first law of thermodynamic in equation (4):

$$\Delta \mathrm{U} = Q + W \tag{4}$$

Where ΔU is the change in internal energy, Q the heat added to the system and W is the work done on the system by the surrounding. Considering an adiabatic system, the change in the strain of the material is equal to the work done by the testing machine, leading to equation (5):

$$\sum_{elem}^{N} \frac{1}{2} \int_{\Omega_\mathrm{e}} \boldsymbol{\Delta\varepsilon}_e^T \Delta\boldsymbol{\sigma_e} d\Omega_\mathrm{e} = W_i \tag{5}$$

Imposing the strain energy convexity constraints formulated in equation (6):

$$\boldsymbol{\varepsilon}^T \boldsymbol{C\varepsilon} \geq 0 \tag{6}$$

The constitutive equation matrix C must be semi-positive definite, it could be decomposed into the Cholesky triangular matrix L with equation (8):

$$C = LL^T \tag{8}$$

The PINN is designed to predict a positive definite matrix C by predicting the Cholesky triangular matrix L, later used to get the constitutive matrix C.

The aforementioned assumptions restrict the solution domain, enhancing the machine learning capabilities of finding the best weight and bias by training the network on the experimental database. The final formulation of the problem is reported in equation (9):

$$\bar{w},\ \bar{b} = \min_{w,\,b} \sqrt{\sum_i^N \frac{\left(\int_0^{d_i} \boldsymbol{f}\, dx - \frac{\sum_j^{n_x \cdot n_y} t_j A_j \boldsymbol{\varepsilon}_j^T \cdot \mathbb{N}(\boldsymbol{\varepsilon}_j; \boldsymbol{w}, \boldsymbol{b}) \mathbb{N}^T(\boldsymbol{\varepsilon}_j; \boldsymbol{w}, \boldsymbol{b}) \varepsilon}{n_x n_y}\right)^2}{N}} \tag{9}$$

Where n_e is the total number of DIC elements.

2.2.3 Unit-consistent data normalization

It is known that the normalization of input and output data facilitates the training process of Neural Networks. When the gradient of the prediction error is of different order of magnitude respect to the input parameters, the convergence of the optimization algorithm is slow and unstable. More specifically, unscaled input data can slow down the learning process and requires small learning rates, whereas unscaled outputs can results in exploding gradients causing the learning process to fail. The NN designed in this study learns the constitutive equation of composite materials, linking the applied strains, which magnitude is 10^{-4}, to the material stress, with magnitude of 10^{2} (expressed in MPa); thus, the network weights will be in the order of 10^{6}, leading to unstable learning and higher generalization error. The natural conclusion follows that both input and output data should be scaled within the same, small range (e.g., between 0 and 1); however, the structure of the mechanistic PI-NN contains physic equations, whose validity is preserved by the unit consistency. Scaling the data would stretch the strain and energy values, affecting the physical consistency of equation (9):

$$\mathcal{L} = \sum_i^{N_f} \sqrt{\frac{\left(\frac{1}{2}\sum_e^N \int_{\Omega_e} \boldsymbol{\varepsilon}_e^T \boldsymbol{C} \boldsymbol{\varepsilon}_e d\Omega_e - E_i\right)^2}{N_f}} \tag{9}$$

If both the input, $\boldsymbol{\varepsilon}_e$, and the output, E_i, are scaled within the range [0, 1] through equations (10):

$$\bar{\varepsilon}_e = \frac{\varepsilon_e - \varepsilon_{min}}{\varepsilon_{max} - \varepsilon_{min}};\quad \bar{E}_\iota = \frac{E_i - E_{min}}{E_{max} - E_{min}} \tag{10}$$

For each frame, the error will be computed by equation (11) as:

$$\frac{1}{2}\sum_e \int_{\Omega_e} \bar{\varepsilon}_e^T C \bar{\varepsilon}_e\, d\Omega_e - \bar{E}_\iota \tag{11}$$

Where the left and right term are no longer compliant in units. To overcome this issue, while both preserving the advantage of scaling the database and preserving the physical meaning of the mechanistic PI-NN, the network is passing the scaled input only to the layers predicting the constitutive law. The computation of the loss function is performed with the unscaled values and the predicted energy is later scaled consistently with the output, yielding to equations (12).

$$\bar{E}_i^{pred} = \frac{\frac{1}{2}\sum_e^N \int_{\Omega_e} \boldsymbol{\varepsilon}_e^T \boldsymbol{C}(\bar{\boldsymbol{\varepsilon}}_e) \boldsymbol{\varepsilon}_e d\Omega_e}{E_{max}} \tag{12}$$

$$\mathcal{L} = \sum_i^{N_f} \sqrt{\frac{(\bar{E}_i^{pred} - \bar{E}_i)^2}{N_f}}$$

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Since every test starts from the undeformed configuration with zero load applied, E_{min} is equal to zero and the constitutive matrix C can be rescaled to restore the real units.

2.2.4 Neural network structure

Once the optimization problem for the training of the PINN has been defined, the network is built stacking multiple layers of neurons as described in Table (1).

Table 1: Neural Network structure.

Layer	Type	Neurons	Activation function	Output dimension
1	Input	0	-	(3, 1)
2	Normalization	0	-	(3, 1)
3	Dense	10	Linear	(10, 1)
4	Physic	10	Linear	(4, 1)
5	Reshape	0	-	(3, 3)

4. Results

As discussed in Section 3, the proposed PINN is not learning a material law from a ground truth stress measurements, hence a direct comparison with the reference stress can not be analysed. Figure 4 shows the training curve of the PINN trained on the A20_1 specimen on the left, and the variation of the term of the constitutive matrix in position (3,3) with the shear strain on the right.

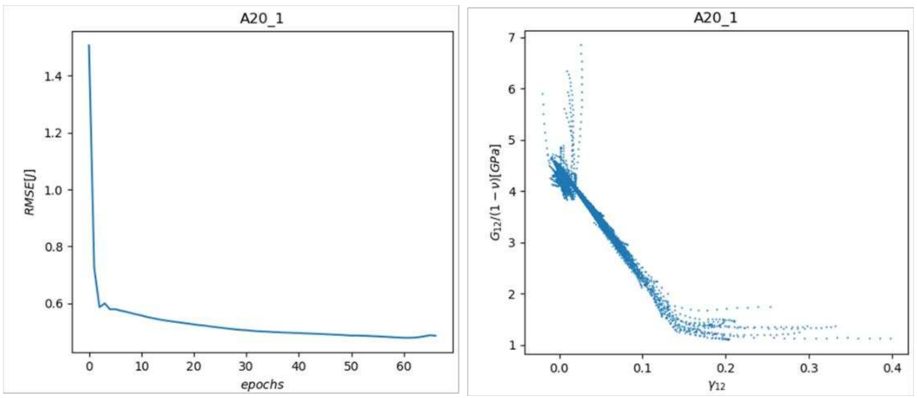

Figure 4. On the left, the training history of the PINN; on the right, the variation of the shear term of the constitutive matrix with the applied shear strain.

The regression error on the prediction of the variation of internal energy is lower than 0.5 J over a total energy variation of 35 J. From the angle-ply tensile test, the networks learned a damage law with a linear degradation of the shear modulus, until a plateau of residual stiffness of 1 GPa after an engineering shear strain of 0.15 . The right graph on Figure 4 shows the capability of the PINN to learn a material law accounting for the local strain state of each element in the structure.

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