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Damage-enhanced order reduction models for woven composites based on data-driven multiscale mechanics

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Abstract — An innovative data-driven homogenization method called Deep Material Network (DMN) was recently proposed in the literature and has shown its advantages in efficiently approximating complex mechanical behaviours of heterogeneous materials. Along the same line, three *ad hoc* Reduced-Order Models (ROMs) were then developed with the aim of making the DMN approach more adaptive to the structural characteristics of woven composites. In this work, the previous proposed ROMs for woven composites are enhanced by taking into account the damage and failure process in their different phases.
Mots clés — woven composites, reduced order model, damage.

1 Introduction

For the last few decades, woven fabric composites have emerged as an innovative solution to reduce the mass of structural components with complex shapes while improving their mechanical performance, and they are now widely used in the aerospace, automotive and marine industries. However, the architectural complexity combined with the multi-scale heterogeneities of this type of material give rise to many difficulties concerning the prediction of its local and global responses, especially after the onset of various energy-dissipating mechanisms collectively referred to as plasticity or damage. Therefore, a physically accurate and numerically efficient modelling for such materials across different scales is a scientific challenge and has been the subject of many research works in recent years. From now on, with the developments lately carried out around various analytical, semi-analytical or numerical homogenization methods, it is possible to determine equivalent effective properties in linear elasticity for a heterogeneous microstructure by the definition of a Representative Unit Cell (RUC) at a given meso-scale. Nevertheless, in non-linear inelastic regime, these methods suffer from various drawbacks in terms of precision and / or of computational efficiency.

In the context of heterogeneous materials, an innovative data-driven homogenization method called Deep Material Network (DMN) was recently proposed in [1], and has shown its interesting advantages in correctly approximating complex linear or non-linear mechanical behaviours of a heterogeneous material throughout the construction of a network of mechanistic building blocks. Inspired by the principle of machine learning and using mathematical and computational tools related to data science, the DMN is composed of mechanistic building blocks distributed in the form of a tree structure (an example is shown in Figure 1 for a two-phase material, in which the nodes in red and in blue of the deepest layer represent different phases), and is governed by a reduced number of degrees of freedom to be identified. Like all classical networks, this identification (often called offline training) is done by solving an optimization problem: we seek to minimize a loss function which measures the distances between the reference values given, for example, by a high-fidelity model, and the solutions resulting from the considered surrogate model. But unlike other networks such as neural networks, the identification of a DMN only requires reference values obtained in a linear elastic regime. Indeed, one of the advantages of this new methodology lies in its ability to extrapolate outside the database used for its training, which not only allows to accelerate the computational time, but also to reduce the required memory. The interested reader is referred to [2] for more detailed theoretical analyses related to this method, and some of its applications on composite materials can be found in [3, 4].

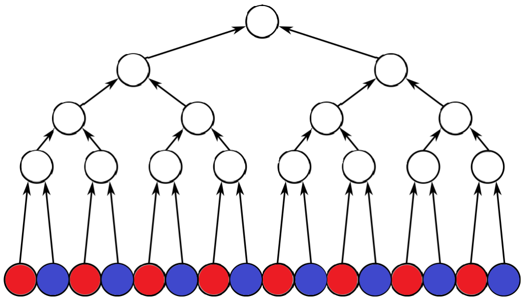
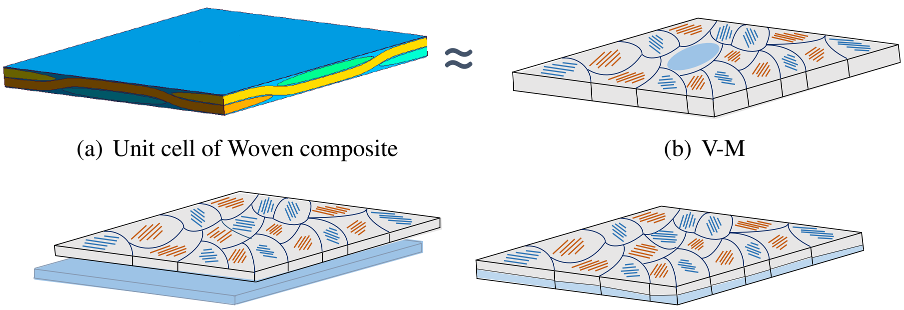


Figure 1: Sketch of a DMN for a two-phase material.

2 Reduced order models for woven composite RUC elastic property estimations

Motivated by this very promising new approach based on data science, the CM3 laboratory then proposed along the same line in [5] three *ad hoc* Reduced-Order Models (ROMs) , respectively named Voigt-Mean-Field Homogenization (MFH) (or VM), Laminate-Voigt-MFH (or LVM) and Voigt-Laminate-MFH (or VLM), with the aim of making the DMN approach more efficient with respect to the structural characteristics of 2D woven composites. As illustrated in Figure 2, the three ROMs assimilate a RUC in woven composite to mechanistic pseudo-grains in pure matrix or in short fibres reinforced matrix, and are parametrized only by a small number of topological parameters such as the aspect ratios and the orientation angles of the short fibres, as well as the volume fractions and the rotation angles of the pseudo-grains. In addition, the interaction of the latter is efficiently introduced by combinations of different analytical or semi-analytical homogenization methods (*e.g.* Voigt's rule of mixture, MFH method) and the theory of laminates.



(a) Unit cell of Woven composite (b) V-M (c) LVM (d) VLM

Figure 2: Woven composites approximation proposed in [5]: (a) a woven composite RUC is successively approximated (b) by an aggregate of pseudo-grains of pure matrix and of short fibre reinforced matrix (VM); or (c) by a laminate of two plies respectively made of a pure matrix and of an aggregate of pseudo-grains of short fibre reinforced matrix (LVM); or again (d) by an aggregate of pseudo-grains of 2-ply laminates made of pure matrix and of short fibre reinforced matrix (VLM).

2.1 Voigt-MFH (VM) scheme

The first ROM is constructed by following a Voigt-MFH (VM) scheme as shown in Figure 2(b). In this scheme, the woven composite RUC is approximated by an aggregate of one pure matrix pseudo-grain representing the pure matrix part (*i.e.* the out of the yarns phase) in a RUC with the corresponding known volume fraction v_0, and N_s short fibre reinforced matrix pseudo-grains representing the yarns in a RUC with the corresponding known fibre volume fraction $V_\mathrm{I} = V_\mathrm{I}^{\mathrm{yarn}}$, but with different volume fractions $\{v_i\}_{1\leq i\leq N_\mathrm{s}}$ (satisfying $\sum_{i=1}^{N_\mathrm{s}} v_i = 1.0 - v_0$), fibre orientations $\{\theta_i\}_{1\leq i\leq N_\mathrm{s}}$ and aspect ratios $\{\alpha_i\}_{1\leq i\leq N_\mathrm{s}}$.

Then, the associated material network can be described in a tree-structure of depth two (see Figure 3), and the homogenised response of the woven composite RUC can be computed by following a twostep bottom-to-top process: firstly, the MFH is carried out on the lowest fibres and matrix nodes to obtain the short fibre reinforced matrix pseudo-grains elasticity tensors $\{\mathbb{C}_i\}_{1\leq i\leq N_s}$; secondly, applying Voigt's rule of mixtures on the aggregate of the pure matrix pseudo-grain and the short fibre reinforced matrix pseudo-grains leads us to the final homogenised elasticity tensor of the woven composite RUC $\mathbb{C}^{\mathrm{VM}}$.

Therefore, the unknown topological parameters involved in this VM model can be collected in the following vector:

$$\chi^{\mathrm{VM}} = \left\{ v_i, \boldsymbol{\theta}_i, \alpha_i \mid i = 1, \ldots, N_s; \sum_{i=1}^{N_s} v_i = 1.0 - v_0 \right\}. \tag{1}$$

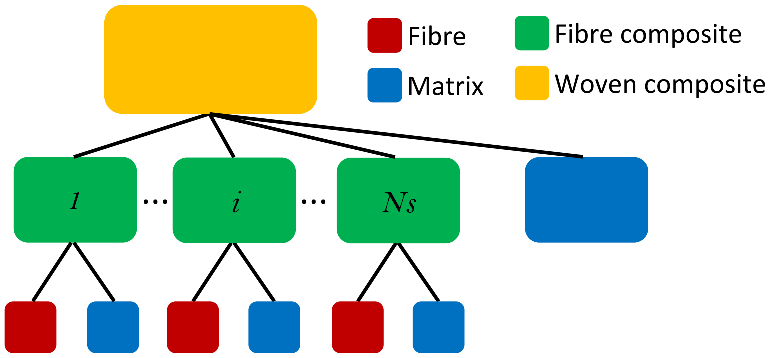


Figure 3: Computational network of the VM scheme.

2.2 Laminate-Voigt-MFH (LVM) scheme

The second ROM is constructed by following a Laminate-Voigt-MFH (LVM) scheme as shown in Figure 2(c). In this scheme, instead of treating the pure matrix part outside of the yarns as a pseudo-grain in Voigt's mixture rule, we approximate it as a ply of a two-ply laminate (respectively referred to by the subscripts A and B) with the corresponding known volume fraction $v_B = v_0$. Consequently, the other ply of the laminate representing the yarns of the RUC is constituted by N_s short fibre reinforced matrix pseudo-grains, with a known volume fraction $v_A = 1 - v_0$. Similar to the VM scheme, these pseudo-grains are parametrized by the corresponding known fibre volume fraction $V_{\mathrm{I}} = V_{\mathrm{I}}^{\mathrm{yarn}}$, and by different volume fractions $\{v_i\}_{1\leq i\leq N_s}$ (satisfying $\sum_{i=1}^{N_s} v_i = 1.0$), fibre orientations $\{\boldsymbol{\theta}_i\}_{1\leq i\leq N_s}$ and aspect ratios $\{\alpha_i\}_{1\leq i\leq N_s}$.

Accordingly, the associated material network can be described in a tree-structure of depth three (see Figure 4), and the homogenised response of woven composite RUC can be computed by following a three-step bottom-to-top process: firstly, like in the VM model, the MFH is carried out on the deepest fibres and matrix nodes to obtain the short fibre reinforced matrix pseudo-grains elasticity tensors $\{\mathbb{C}_i\}_{1\leq i\leq N_s}$; secondly, Voigt's rule of mixture is used on the aggregate of pseudo short fibre reinforced matrix grains, yielding the elasticity tensor of the yarns ply $\mathbb{C}_{\mathrm{A}}$; finally, applying the laminate theory on the pure matrix ply (with a elasticity tensor equals to the one of pure matrix $\mathbb{C}_{\mathrm{B}} = \mathbb{C}_0$) and the yarns ply, we obtain easily the homogenised elasticity tensor of the woven composite RUC $\mathbb{C}^{\mathrm{LVM}}$.

Once again, the unknown topological parameters involved in this LVM model are gathered in a vector:

$$\chi^{\mathrm{LVM}} = \left\{ v_i, \boldsymbol{\theta}_i, \alpha_i \mid i = 1, \ldots, N_s; \sum_{i=1}^{N_s} v_i = 1.0 \right\}. \tag{2}$$

2.3 Voigt-Laminate-MFH (VLM) scheme

The third ROM is constructed by following a Voigt-Laminate-MFH (VLM) scheme as shown in Figure 2(d). In this scheme, the woven composite RUC is approximated by an aggregate of N_s two-ply laminate pseudo-grains, in which a pure matrix ply and a yarns ply are considered for each pseudo-grain. For each two-ply laminate pseudo-grain, it is characterized by an unknown orientation angles vector

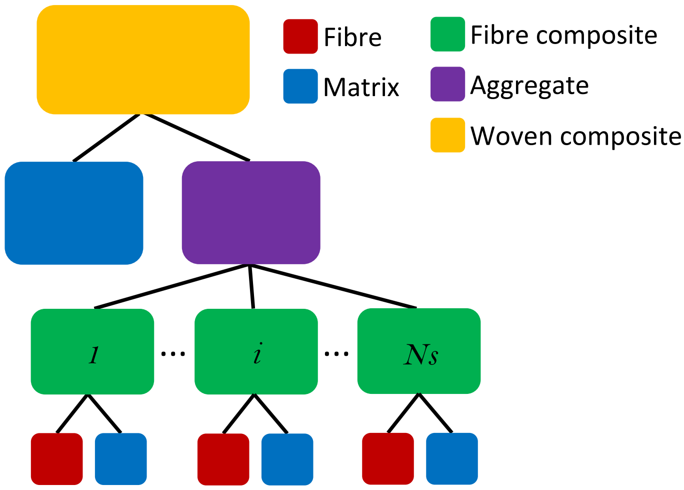


Figure 4: Computational network of the LVM scheme.

$\{\boldsymbol{\theta}_i^{\mathrm{g}}\}_{1\leq i\leq N_{\mathrm{s}}}$, and an unknown volume fraction $\{v_i^{\mathrm{g}}\}_{1\leq i\leq N_{\mathrm{s}}}$ satisfying $\sum_{i=1}^{N_{\mathrm{s}}} v_i^{\mathrm{g}} = 1$. The pure matrix ply, representing the out-of-yarn matrix part in the RUC, is defined by an unknown volume fraction $\{v_i^{\mathrm{m}}\}_{1\leq i\leq N_{\mathrm{s}}}$ satisfying $\sum_{i=1}^{N_{\mathrm{s}}} v_i^{\mathrm{g}} v_i^{\mathrm{m}} = v_0$; while the short fibre reinforced matrix material (yarns) ply, representing the yarns in the RUC, is parametrized by the corresponding known fibre volume fraction $V_{\mathrm{I}} = V_{\mathrm{I}}^{\mathrm{yarn}}$, and by an unknown fibre orientation $\{\boldsymbol{\theta}_i^{\mathrm{f}}\}_{1\leq i\leq N_{\mathrm{s}}}$ as well as an unknown aspect ratio $\{\alpha_i\}_{1\leq i\leq N_{\mathrm{s}}}$ (the volume fraction of the yarns ply can be directly deduced from the volume fraction of the pure matrix ply: $\{v_{\mathrm{A}i} = 1.0 - v_i^{\mathrm{m}}\}_{1\leq i\leq N_{\mathrm{s}}}$).

Then, the associated material network can be described in a tree-structure of depth three (see Figure 5), and the three-step bottom-to-top homogenisation process is as follows: firstly, the MFH is carried out on the lowest fibres and matrix nodes to obtain the short fibre reinforced matrix plies elasticity tensors $\{\mathbb{C}_i\}_{1\leq i\leq N_{\mathrm{s}}}$; secondly, applying the laminate theory on the pure matrix ply (with the elasticity tensor equals to the one of pure matrix $\mathbb{C}_{\mathrm{B}} = \mathbb{C}_0$) and the yarn ply (with the elasticity tensor $\mathbb{C}_{\mathrm{A}i}$ determined by $\mathbb{C}_i$ and $\boldsymbol{\theta}_i^{\mathrm{f}}$), we obtain easily the homogenised elasticity tensors for the two-ply laminate pseudo-grains $\{\mathbb{C}_{\mathrm{L}i}\}_{1\leq i\leq N_{\mathrm{s}}}$; finally, the homogenised elasticity tensor of the woven composite RUC $\mathbb{C}^{\mathrm{VLM}}$ is given by using the Voigt's rule of mixture on the aggregate of two-ply laminate pseudo-grains.

In like manner, the unknown topological parameters vector for this VLM model can be subsequently formed:

$$\boldsymbol{\chi}^{\mathrm{VLM}} = \left\{ v_i^{\mathrm{g}}, \boldsymbol{\theta}_i^{\mathrm{g}}, v_i^{\mathrm{m}}, \boldsymbol{\theta}_i^{\mathrm{f}}, \alpha_i \mid i = 1, \ldots, N_{\mathrm{s}};\ \sum_{i=1}^{N_{\mathrm{s}}} v_i^{\mathrm{g}} = 1.0;\ \sum_{i=1}^{N_{\mathrm{s}}} v_i^{\mathrm{g}} v_i^{\mathrm{m}} = v_0 \right\}. \tag{3}$$

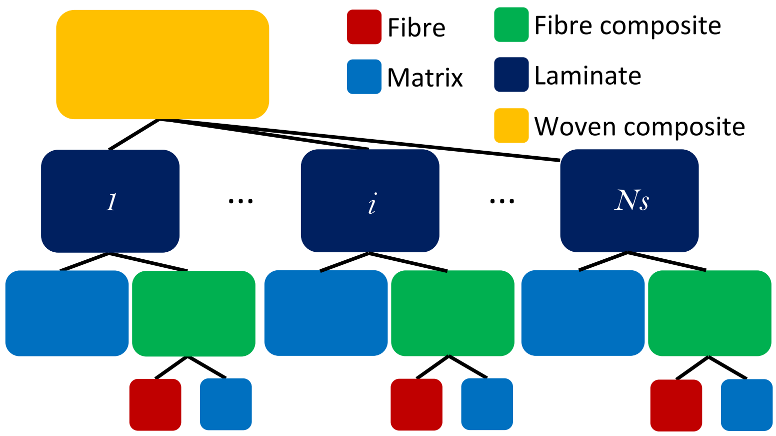


Figure 5: Computational network of the VLM scheme.

3 Offline training of the reduced order models

The identification of the unknown topological parameters vector χ (*e.g.* χ^{VM}, χ^{LVM} and χ^{VLM}) is formulated as a optimization problem during a offline training phase, that consists in minimizing a loss function $L(\hat{\mathbb{C}}, \mathbb{C}(\chi))$:

$$\chi^{\mathrm{opt}} = \arg\min_{\chi} L(\hat{\mathbb{C}}, \mathbb{C}(\chi)), \tag{4}$$

for which the optimal parameters χ^{opt} correspond to the optimal values of the topological parameters χ defined by Eqs. (1), (2) or (3) respectively for the VM, LVM or VLM model. Starting from physically meaningful initial guess of the parameters vector χ, a Stochastic Gradient Descent (SGD) algorithm with Adaptive Moment Estimation (Adam) is adopted for the parameters update.

In our case, the loss function is defined as the evaluation of the distance between the so-called training data which correspond to n realizations of the homogenised elasticity tensor obtained by the direct computational homogenisation on the woven composite RUC $\hat{\mathbb{C}}(\gamma)$ (with γ the material properties vector), and the same number of realizations of the homogenised elasticity tensor obtained by the three proposed models $\mathbb{C}(\chi|\gamma_s) = \mathbb{C}^{\mathrm{VM}}(\chi^{\mathrm{VM}}|\gamma)$, $\mathbb{C}^{\mathrm{LVM}}(\chi^{\mathrm{LVM}}|\gamma)$ or $\mathbb{C}^{\mathrm{VLM}}(\chi^{\mathrm{VLM}}|\gamma)$. Thus, the loss function can be defined as:

$$L(\hat{\mathbb{C}}, \mathbb{C}(\chi)) = \frac{1}{n}\sum_{s=1}^{n} \frac{\|\hat{\mathbb{C}}(\gamma_s) - \mathbb{C}(\chi|\gamma_s)\|}{\|\hat{\mathbb{C}}(\gamma_s)\|} + \frac{\lambda}{2}G(\chi), \tag{5}$$

where $\| \bullet \|$ refers to the Frobenius norm, and the Lagrange multiplier λ is used to enforced the volume fraction consistency expression $G(\chi)$ (see [5] for more details).

4 Online evaluation of the reduced order models

Once the topological parameters vector χ is identified by the offline training process, the corresponding material network is then completely defined, and non-linear inelastic analyses taking into account the plasticity as well as the damage and failure process can be performed according to the information paths and the related computation operations. The matrix phase is assumed to be a J_2 elasto-plastic material, while a transverse isotropic elastic model is used to describe the mechanical behaviour of the fibre phase.

Following the top-to-bottom information paths of the material network, the strain increment is firstly distributed from a parent material node to its descendant nodes at each network level, until reaching the matrix and fibre phases at the bottom of the network. According to the material model type (MFH, Voigt's rule of mixtures or two-ply laminate theory) of the parent nodes, different strain increment distribution rules are adopted. Then, starting from the lowest matrix and fibre material level, the stresses and internal variables of the parent material nodes can be computed from their direct descendant material nodes by solving a series of non-linear equations. Iterations are normally needed between parent and descendant nodes, until the required non-linear equation at the highest material node is balanced. More details concerning these non-linear analyses in online evaluation can be found in [5].

We note also that, in this work, different damage evolution models are also embedded in the MFH process for both matrix and fibre phases (the interested reader is referred to [6] for technical details):

- a deterministic saturation damage law is introduced for the matrix, and the damage variable D_0 can be computed by Eq. (6):

$$D_0 = \frac{D_{\max}}{1 - \frac{1}{1+\exp(sp_{\mathrm{C}})}} \left(\frac{1}{1+\exp(-s(p-p_{\mathrm{C}}))} - \frac{1}{1+\exp(sp_{\mathrm{C}})} \right), \tag{6}$$

  where $D_{\max}$ is the saturation damage, s and p_{C} are two material parameters, and p is the equivalent plastic strain;

- a stochastic damage law is adopted for the fibres, in which the strength of a single fibre can be described using a Weibull function:

$$\Phi(\hat{\sigma}, L) = 1.0 - \exp\left[-\left(\frac{L}{L_0}\right)^{\alpha} \left(\frac{\hat{\sigma}}{\sigma_0}\right)^{m} \right], \tag{7}$$

where $\Phi(\hat{\sigma}, L)$ is the cumulative probability of failure for a fibre with a gauge length L at a given stress level of $\hat{\sigma}$. The scale parameter σ_0 and the shape parameters α and m are related to the material and need to be determined experimentally at the reference gauge length L_0. Therefore, based on this statistical strength distribution assumption, the damage variable D_{I} for a fibre bundle can be computed by Eq. (8):

$$D_{\mathrm{I}} = \varphi + \rho\sqrt{\frac{\varphi(1-\varphi)}{N}}\,, \tag{8}$$

where N is the number of fibres in a fibre bundle, and $\varphi = \Phi\left(\frac{\sigma}{1-D_{\mathrm{I}}}, L\right)$ with σ is the apparent longitudinal loading stress of the fibre bundle.

5 Verification

The accuracy and efficiency of the proposed VM, LVM and VLM models in elasto-plastic regime without considering the damage and failure process has already been verified in [5], by comparing their predictions of the non-linear behaviour of two woven composite RUCs with the reference results obtained by direct numerical simulations in [6]. For their validation in damage-enhanced elasto-plastic regime, only a RUC with 64.56% of yarn volume fraction under Mixed Boundary Condition is examined in the present work. The topological parameters χ^{opt} previously identified respectfully for the three proposed models are reused, and the reference direct finite element results can also be found in [6]. Moreover, we note that the damage evolution laws used for both matrix and fibres in [6] are non-local models in order to remove the mesh dependency. Nevertheless, these non-local formulations loss their physical meanings for our proposed ROMs, since inside each pseudo-grains damage evolution should be homogenous. Thus, their local forms are used instead as presented in Eq. (6) and Eq. (8), and their parameters are evaluated from a virtual test with non-local damage models to have a similar response. Figure 6 shows that, for a unidirectional tensile test, the VM and VLM models capture well not only the macro stress but also the global failure point in comparison to the direct finite element results, but for the LVM model we observe a premature failure even its strain-stress curve overlaps with the other two models and the reference results with little discrepancy.

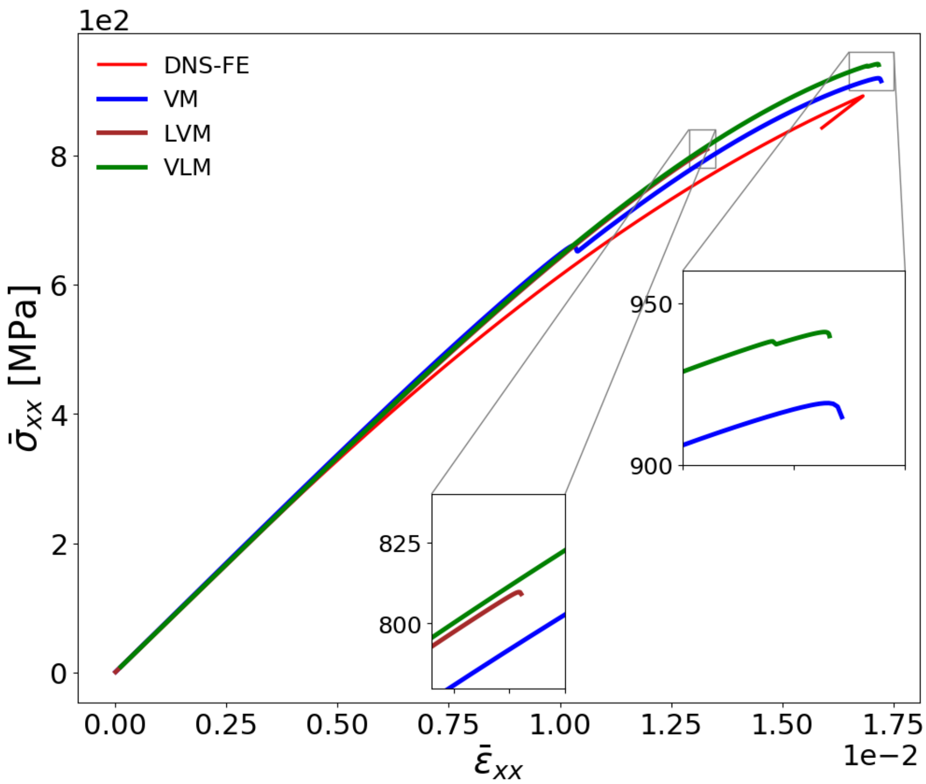


Figure 6: Uniaxial tensile test on the RUC

6 Conclusions and perspectives

By introducing suitable damage evolution laws for both matrix and fibre phases, we extend three material network based reduced-order models, previously constructed and trained in linear elasticity for woven composite materials, into damage-enhanced non-linear elasto-plasticity. The validity of the proposed models has been examined by comparing their predictions with direct numerical simulations on a woven composite RUC, and the performance of the VM and VLM models is satisfactory. In the future work, the presented methodology will be improved to be able to adapt to 3D composite structures.

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