Damage-enhanced order reduction models for 2D woven composites based on data-driven multiscale mechanics

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Context

2D woven composites

- periodic heterogeneous multiscale materials that can be described by RVEs
 - mesoscale ($\sim 10^{-3}$ m) RVE: matrix + warp and weft yarns
 - microscale ($\sim 10^{-6}$ m) RVE of yarns: UD fibres + matrix
- damage-enhanced nonlinear behaviours for constituents
 - fibres: transversely isotropic linear elasticity
 - matrix: isotropic J₂ elasto-plasticity
- numerical modelling and simulation
 - complex geometrical description and material properties assignment
 - high computational cost (time and memory usage)



Figure: Multiscale description of a 2D woven composite [Wang et al. 2017]

Context

Mean-Field Homogenisation (MFH) for yarns

• semi-analytical solution for the extended Eshelby problem with multiple inclusions

$$\bar{\boldsymbol{\varepsilon}} = v_{\mathbf{I}} \boldsymbol{\varepsilon}_{\mathbf{I}} + v_0 \boldsymbol{\varepsilon}_0 , \quad \bar{\boldsymbol{\sigma}} = v_{\mathbf{I}} \boldsymbol{\sigma}_{\mathbf{I}} + v_0 \boldsymbol{\sigma}_0$$

• Linear Comparison Composite (LCC)-based nonlinear framework

$$\Delta \boldsymbol{\varepsilon}_{\mathsf{I}} = \mathbb{B}^{\epsilon} \left(\mathsf{I}, \, \mathbb{C}_{\mathsf{I}}^{\mathsf{LCC}}, \, \mathbb{C}_{0}^{\mathsf{LCC}} \right) : \Delta \boldsymbol{\varepsilon}_{0}$$

• Mori-Tanaka (MT) model

$$\mathbb{B}^{\varepsilon}\left(I,\,\mathbb{C}_{I}^{LCC},\,\mathbb{C}_{0}^{LCC}\right) = \left\{\mathbb{I} + \mathbb{S}\left(I,\,\mathbb{C}_{0}^{LCC}\right) : \left[\left(\mathbb{C}_{0}^{LCC}\right)^{-1}:\mathbb{C}_{I}^{LCC} - \mathbb{I}\right]\right\}^{-1}$$

Context

Full-order FE modelling and damage-enhanced MFH-based nonlinear Direct Numerical Simulation (DNS) ([Wu, Maillard, and Noels 2021] and [Wu et al. 2021])

- computational cost: 63189 elements; ~ 3 days
- still too high for applications of industrial complexity



Figure: FE model of a 2D woven RVE at mesoscale

Propose a reduced-order model (ROM) for 2D woven composites by embedding

- micromechanics-based homogenization methods
- data-driven model reduction techniques

to conduct accurately and efficiently damaged-enhanced nonlinear multiscale analysis

Outline

Introduction

- 2 Reduced-order models
- Offline training and online evaluation
- Application
- Conclusions and outlooks

Outline

Introduction

2 Reduced-order models

- Deep Material Network (DMN)
- VM scheme
- LVM scheme
- VLM scheme

3 Offline training and online evaluation

Application

6 Conclusions and outlooks

Deep Material Network (DMN)

Deep Material Network (DMN) [Liu and Wu 2019]: a ROM for RVE

- mechanistic building blocks-based tree structure: homogenization + rotation
- efficient offline training in linear elastic regime: geometrical parameters fitting
- accurate online extrapolation in arbitrary unknown nonlinear inelastic regime: mechanical response prediction



Figure: Illustration of a 3-layer DMN for a biphasic material

VM scheme

DMN-liked VM scheme [Wu, Adam, and Noels 2021]: 2D woven RVE \approx Short Fibre Reinforced Matrix (SFRM) pseudo-grains aggregate



- step 1: matrix + fibres \Rightarrow MFH \Rightarrow SFRM
- step 2: SFRMs \Rightarrow Voigt's rule of mixtures \Rightarrow 2D woven RVE
- parameters: $\boldsymbol{\chi}^{\mathsf{VM}} = \left\{ v_i, \, \boldsymbol{\theta}_i, \, \alpha_i \mid i = 1, ..., N_{\mathsf{s}}; \, \sum_{i=1}^{N_{\mathsf{s}}} v_i = 1.0 v_0 \right\}$



Figure: Illustration of the VM scheme $(N_s = 3)$

LVM scheme

DMN-liked LVM scheme [Wu, Adam, and Noels 2021]: 2D woven RVE \approx 2-ply laminate



- step 1: matrix + fibres \Rightarrow MFH \Rightarrow SFRM
- step 2: SFRMs \Rightarrow Voigt's rule of mixtures \Rightarrow SFRMs aggregate
- step 3: matrix ply + aggregate ply \Rightarrow Laminate theory \Rightarrow 2D woven RVE
- parameters: $\boldsymbol{\chi}^{\text{LVM}} = \left\{ v_i, \boldsymbol{\theta}_i, \alpha_i \mid i = 1, ..., N_{\text{s}}; \sum_{i=1}^{N_{\text{s}}} v_i = 1.0 \right\}$



Figure: Illustration of the LVM scheme $(N_s = 3)$

VLM scheme

DMN-liked VLM scheme [Wu, Adam, and Noels 2021]: 2D woven RVE \approx 2-ply laminate pseudo-grains aggregate



- step 1: matrix + fibres \Rightarrow MFH \Rightarrow SFRM
- step 2: matrix ply + SFRM ply \Rightarrow Laminate theory \Rightarrow 2-ply laminate
- step 3: 2-ply laminate aggregate \Rightarrow Voigt's rule of mixtures \Rightarrow 2D woven RVE

• parameters:
$$\boldsymbol{\chi}^{\text{VLM}} = \left\{ v_i^{\text{g}}, \, \boldsymbol{\theta}_i^{\text{g}}, \, v_i^{\text{m}}, \, \boldsymbol{\theta}_i^{\text{f}}, \, \alpha_i \mid i = 1, ..., N_{\text{s}}; \, \sum_{i=1}^{N_{\text{s}}} v_i^{\text{g}} = 1.0; \, \sum_{i=1}^{N_{\text{s}}} v_i^{\text{g}} v_i^{\text{m}} = v_0 \right\}$$



Figure: Illustration of the VLM scheme $(N_s = 3)$

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Offline training

Identification of χ^{opt} in linear elasticity by solving

$$oldsymbol{\chi}^{\mathsf{opt}} = rg\min_{oldsymbol{\chi}} L(\hat{\mathbb{C}}(oldsymbol{\gamma}), \, ar{\mathbb{C}}(oldsymbol{\chi}|oldsymbol{\gamma}_s))$$

with

- $\hat{\mathbb{C}}(\gamma)$: homogenized elasticity tensor given by computational homogenization on a full-order model parametrized by $\gamma = (E_0, \nu_0, E_l^{\mathsf{T}}, E_l^{\mathsf{L}}, \nu_l^{\mathsf{LT}}, \nu_l^{\mathsf{TT}}, G_l^{\mathsf{LT}})$
- $\mathbb{C}(\chi|\gamma_s)$: homogenized elasticity tensor given by VM, LVM or VLM scheme parametrized by $\chi^{\rm VM}$, $\chi^{\rm LVM}$ or $\chi^{\rm VLM}$ for given γ
- loss function: ($G(\boldsymbol{\chi})$ is a volume fraction consistency function)

$$L(\hat{\mathbb{C}}, \, \bar{\mathbb{C}}(\boldsymbol{\chi})) = \frac{1}{n} \sum_{s=1}^{n} \frac{\|\hat{\mathbb{C}}(\boldsymbol{\gamma}_{s}) - \bar{\mathbb{C}}(\boldsymbol{\chi}|\boldsymbol{\gamma}_{s})\|}{\|\hat{\mathbb{C}}(\boldsymbol{\gamma}_{s})\|} + \frac{\lambda}{2} G(\boldsymbol{\chi})$$

Online evaluation

Extrapolation to unknown material and loading spaces: NR iterative resolution for nonlinear equations

- top-bottom backward de-homogenisation process
- bottom-top forward homogenisation process



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3 Offline training and online evaluation

Application

- Uniaxial tensile test and shear test
- Local damage models calibration
- Damage-enhanced uniaxial tensile test

5 Conclusions and outlooks

Uniaxial (cyclic) tensile test & In-plane cyclic shear test

- training results is available in [Wu, Adam, and Noels 2021]
- damage-free nonlinear predictions with
 - fibres: transversely isotropic linear elasticity
 - matrix: isotropic J_2 elasto-plasticity



Figure: Uniaxial tensile test

Figure: In-plane shear test

comparison of the CPU time

	Tensile	Shear
DNS	11 h	76 h
VM	30 s	$22 \ \mathrm{s}$
LVM	35 s	$25 \ \mathrm{s}$
VLM	35 s	22 s

Uniaxial (cyclic) tensile test & In-plane cyclic shear test

• comparison of the global responses for the uniaxial tensile (cyclic) test



• comparison of the global responses for the in-plane cyclic shear test



Local damage models calibration

Non-local damage models are used for DNS

• phase field-liked damage model for fibres, Lemaitre-like damage model for matrix [Wu et al. 2021]

Local damage models are used for VM, LVM and VLM

- no physical "characteristic length" between material nodes
- Weibull-like damage model for fibres, Lemaitre-like damage model for matrix [Wu, Maillard, and Noels 2021]

Calibration with an uniaxial tensile test on a UD composite sample



Damage-enhanced uniaxial tensile test - Load until failure

Comparison of the global responses

	Strength
	[GPa]
DNS	891.778
VM	892.981
rel. err. (%)	0.13
LVM	852.096
rel. err. (%)	4.45
VLM	913.868
rel. err. (%)	2.48



LVM training results and responses of the two plies

- Aggregate ply takes the majority load
- $\bullet\,$ Grains 9, 10, 19 and 20 have a small $\alpha\,$



Grain	α
1 (weft) & 2 (warp)	216.645
3 (weft) & 4 (warp)	258.721
5 (weft) & 6 (warp)	195.969
7 (weft) & 8 (warp)	181.194
9 (weft) & 10 (warp)	21.032
11 (weft) & 12 (warp)	247.153
13 (weft) & 14 (warp)	204.540
15 (weft) & 16 (warp)	123.377
17 (weft) & 18 (warp)	298.981
19 (weft) & 20 (warp)	23.852



Matrix and fibres damage evolution in the grains of the aggregate ply:



- Deactivation of matrix damage in
 - $\bullet~$ VM: grains 2~ and 3~
 - LVM: grains 9, 10, 19 and 20
- Comparison of the global responses:

	Strength [GPa]	CPU Time
DNS	891.778	64 h
VM	892.981	
rel. err. (%)	0.13	10 s
VM-Mod.	931.430	13 5
rel. err. (%)	4.45	
LVM	852.096	
rel. err. (%)	4.45	6 mins
LVM-Mod.	918.646	0 mins
rel. err. (%)	3.01	
VLM	913.868	17 mins
rel. err. (%)	2.48	17 111115



Comparison of matrix damage state • DNS



Comparison of fibres damage state (DNS vs. VM)



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Conclusions and outlooks

Conclusions

- Construction of DMN-liked and micromechanics-based damage-enhanced ROMs (VM, LVM and VLM) for 2D woven composites
- Efficient offline learning only in linear elasticity
- Accurate online extrapolation to arbitrary unknown nonlinear inelastic material laws and loading spaces

Outlooks

- Improvement of the accuracy by considering more suitable damage models
- Application for 3D woven composites and for other types of composites

Thanks for your attention !

References I

Liu, Z. and C. Wu (2019). "Exploring the 3D architectures of deep material network in data-driven multiscale mechanics". In: *Journal of the Mechanics and Physics of Solids* 127, pp. 20–46.

Sun, Z. et al. (2020). "Numerical analysis of out-of-plane thermal conductivity of C/C composites by flexible oriented 3D weaving process considering voids and fiber volume fractions". In: *Journal of Materials Research* 35.14, pp. 1888–1897.



Wang, L. et al. (2017). "Progressive failure analysis of 2D woven composites at the meso-micro scale". In: *Composite structures* 178, pp. 395–405.

Wu, L., L. Adam, and L. Noels (2021). "Micro-mechanics and data-driven based reduced order models for multi-scale analyses of woven composites". In: *Composite Structures* 270, p. 114058.



Wu, L., E. Maillard, and L. Noels (2021). "Tensile failure model of carbon fibre in unidirectionally reinforced epoxy composites with mean-field homogenisation". In: *Composite Structures* 273, p. 114270.



Wu, L. et al. (2021). "Per-phase spatial correlated damage models of UD fibre reinforced composites using mean-field homogenisation; applications to notched laminate failure and yarn failure of plain woven composites". In: *Computers & Structures* 257, p. 106650.

Appendix A.1 - Damage models for fibre bundle

Local damage evolution (VM, LVM or VLM)

$$D_{\mathsf{I}} = \varphi + \varrho \sqrt{\frac{\varphi(1-\varphi)}{N}}$$

with

- $\varphi(\hat{\sigma}_{I}^{zz}) \sim$ Weibull distribution, with $\hat{\sigma}_{I} = \mathbb{C}_{I}^{el} : \varepsilon_{I}$
- ρ one realisation of $P \sim \mathcal{N}(0, 1)$, and N the number of fibres in a bundle

Non-local damage evolution (full-order model)

$$D_{\mathsf{I}}(x, t) = 1 - (1 - d_{\mathsf{I}}(x, t))^n$$

with

- $d_{I}(x, t)$ given by the phase-field model
- $n \in [2, 3]$ shape parameter

Local (VM, LVM or VLM) and non-local (full-order model) damage evolution

$$D_0 = \frac{D_0^{\max}}{1 - \frac{1}{1 + \exp\{(s_0 p_{\mathsf{C}_0})\}}} \left(\frac{1}{1 + \exp\{(-s_0(\chi_0 - p_{\mathsf{C}_0}))\}} - \frac{1}{1 + \exp\{(s_0 p_{\mathsf{C}_0})\}}\right)$$

with

- D_0^{\max} the saturation damage level
- s_0 and p_{C_0} two material parameters
- $\chi_0(t)$ guarantee of the irreversibility
 - local: $\chi_0(t) = \max_{\tau \in [0, t]} (p_0)$ with $\dot{p}_0 = \sqrt{\frac{2}{3}} \dot{\epsilon}_0^{\mathsf{pl}} : \dot{\epsilon}_0^{\mathsf{pl}}$
 - non-local: $\chi_0(\boldsymbol{x}, t) = \max_{\tau \in [0, t]} (\tilde{p}_0)$ with $\tilde{p}_0 \nabla \cdot (\boldsymbol{c}_0 \cdot \nabla \tilde{p}_0) = p_0$

Information paths for a parent node with N_d direct child nodes

• top-bottom strain distribution:

$$\Delta \boldsymbol{\varepsilon} = \begin{cases} \sum_{i=1}^{N_{\rm d}} v_i^{\rm d} \Delta \boldsymbol{\varepsilon}_i^{\rm d}, & \text{ for MFH-based and 2-ply laminate-based node} \\ \{\Delta \boldsymbol{\varepsilon}_i^{\rm d}\}_{i=1,\ldots,N_{\rm d}}, & \text{ for Voigt's mixtures-based node} \end{cases}$$

• bottom-top stress and algorithmic operator collection:

$$oldsymbol{\sigma} = \sum_{i=1}^{N_{\mathsf{d}}} v_i^{\mathsf{d}} oldsymbol{\sigma}_i^{\mathsf{d}}$$

$$\mathbb{C}^{\mathsf{alg}} = \mathbb{C}^{\epsilon arepsilon} = rac{\mathsf{d} oldsymbol{\sigma}}{\mathsf{d} arepsilon} = \sum_{n=1}^{N_{\mathsf{d}}} v_n^{\mathsf{d}} \mathbb{C}_n^{\mathsf{alg, d}} : rac{\mathsf{d} arepsilon_n^{\mathsf{d}}}{\mathsf{d} arepsilon}$$

Linearisation of the composite parent node by a damage-enhanced incremental-secant-based Linear Comparison Composite (LCC)



Figure: Composite parent node linearisation

• unloading: (*i* for fibre and matrix)



• reloading: (*i* for fibre and matrix)



Linearisation of the fibre child node by a damage-enhanced transversely isotropic elastic material with $E_{\rm I}^{\rm zD} = (1 - D_{\rm I})E_{\rm I}^{\rm z}$ and $\nu_{\rm I}^{\rm zxD} = (1 - D_{\rm I})\nu_{\rm I}^{\rm zx}$



Linearisation of the matrix child node by a damage-enhanced isotropic J_2 elasto-plastic material with $\kappa_0^{\text{D}} = (1 - D_0^n)\kappa_0$, $\mu_0^{\text{D}} = (1 - D_0^n)\mu_0$ and $\mu_0^{\text{SD}} = (1 - D_0^n)\mu_0^{\text{S}} = (1 - D_0^n)(\mu_0 - (3\mu_0^2\dot{p})/(\mathbb{C}_0^{\text{el}} : \Delta\varepsilon_0^{\text{r}})^{\text{eq}})$



Figure: Matrix child node linearisation

7/16

 $\boldsymbol{\varepsilon}_{0}^{n+1} = \boldsymbol{\varepsilon}_{0}^{\text{res},n} + \Delta \boldsymbol{\varepsilon}_{0}^{\text{r}}$ $\boldsymbol{\sigma}_{0}^{n+1} = \boldsymbol{\sigma}_{0}^{\text{res},n} + \mathbb{C}_{0}^{\text{SD}}(D_{0}^{n+1}) : \Delta \boldsymbol{\varepsilon}_{0}^{\text{r}}$

Nonlinear equation for the MFH problem: (S the so-called Eshelby tensor)

$$\mathbf{F}_{\mathsf{MFH}} = \mathbb{C}_{0}^{\mathsf{SD}} : \left[\Delta \boldsymbol{\varepsilon}_{\mathsf{I}}^{\mathsf{r}} - \frac{1}{v_{0}} \mathbb{S}^{-1}(\mathsf{I}, \mathbb{C}_{0}^{\mathsf{SD}}) : (\Delta \boldsymbol{\varepsilon}_{\mathsf{I}}^{\mathsf{r}} - \Delta \boldsymbol{\varepsilon}^{\mathsf{r}}) \right] - \mathbb{C}_{\mathsf{I}}^{\mathsf{SD}} : \Delta \boldsymbol{\varepsilon}_{\mathsf{I}}^{\mathsf{r}}$$

NR iterative resolution: (i for fibre or matrix)



Appendix B.2 - Nonlinear analyses for 2-ply laminate-based node

Nonlinear equation to satisfy for the 2-ply laminate problem:

$$\mathbf{F}_{\mathsf{Lam}} = \begin{bmatrix} (\sigma_{\mathsf{A}}^{\mathsf{zz}} - \sigma_{\mathsf{B}}^{\mathsf{zz}}) + (\varepsilon_{\mathsf{A}}^{\mathsf{xx}} - \varepsilon_{\mathsf{Lam}}^{\mathsf{xx}}) \\ (\sigma_{\mathsf{A}}^{\mathsf{xz}} - \sigma_{\mathsf{B}}^{\mathsf{xz}}) + (\varepsilon_{\mathsf{A}}^{\mathsf{yy}} - \varepsilon_{\mathsf{Lam}}^{\mathsf{yy}}) \\ (\sigma_{\mathsf{A}}^{\mathsf{yz}} - \sigma_{\mathsf{B}}^{\mathsf{yz}}) + (\varepsilon_{\mathsf{A}}^{\mathsf{xy}} - \varepsilon_{\mathsf{Lam}}^{\mathsf{xy}}) \end{bmatrix} = \mathbf{0}$$

NR iterative resolution: (i for A-ply or B-ply)



Appendix B.3 - Nonlinear analyses for Voigt's mixtures-based node

No nonlinear equation to be solved for the Voigt's mixtures problem

VM			
Grain	θ	v	α
1 (matrix)	-	0.3544	-
2 (weft) & 3 (warp)	[0/90, 89.99982, 0]	0.0204	6.469
4 (weft) & 5 (warp)	[0/90, 89.99986, 0]	0.2737	151.095
6 (weft) & 7 (warp)	[0/90, 89.99985, 0]	0.0286	105.591

Grain	θ	v	α
1 (weft) & 2 (warp)	[0/90, 82.432, 0]	0.0314	216.645
3 (weft) & 4 (warp)	$\left[0/90, 90.648, 0 ight]$	0.2618	258.721
5 (weft) & 6 (warp)	$\left[0/90, 90.651, 0 ight]$	0.0770	195.969
7 (weft) & 8 (warp)	$\left[0/90, 93.161, 0 ight]$	0.0241	181.194
<mark>9</mark> (weft) & <mark>10</mark> (warp)	$\left[0/90, 116.875, 0 ight]$	0.0176	21.032
11 (weft) & 12 (warp)	$\left[0/90, 92.995, 0 ight]$	0.0179	247.153
13 (weft) & 14 (warp)	$\left[0/90, 80.612, 0 ight]$	0.0105	204.540
15 (weft) & 16 (warp)	[0/90, 102.166, 0]	0.0073	123.377
17 (weft) & 18 (warp)	$\left[0/90, 88.039, 0 ight]$	0.0312	298.981
19 (weft) & 20 (warp)	$\left[0/90, 66.960, 0 ight]$	0.0211	23.852

LVM

VLM

Grain	$ heta^{ m f}$	$ heta^{ m g}$	v^{m}	v^{g}	α
1 (weft) & 2 (warp)	[0, 89.963, 0]	$\left[0/90, 0.479, 0 ight]$	0.2291	0.2721	152.599
3 (weft) & 4 (warp)	[0, 179.575, 0]	$\left[0/90, -89.584, 0\right]$	0.5216	0.0204	542.078
5 (weft) & 6 (warp)	[0, 89.698, 0]	$\left[0/90, 8.230, 0 ight]$	0.5514	0.0614	285.184
7 (weft) & 8 (warp)	[0, 90.256, 0]	$\left[0/90, -6.628, 0\right]$	0.5073	0.0681	207.968
9 (weft) & 10 (warp)	[0, 90.108, 0]	$\left[0/90,-2.391,0\right]$	0.4424	0.0755	189.845
11 (weft) & 12 (warp)	[0, 90.095, 0]	$\left[0/90, -59.110, 0\right]$	0.9995	0.0024	367.619

Appendix D.1 - Uniaxial tensile test - Load-Unload

Comparison of the global responses:

	Strength CPU Tin	
	[GPa]	[mins]
DNS	831.481	1204
VM	848.241	
rel. err. (%)	2.02	0.05
VM-Mod.	882.647	0.05
rel. err. (%)	6.15	
LVM	851.166	
rel. err. (%)	2.37	1
LVM-Mod.	870.576	1
rel. err. (%)	4.70	
VLM	869.539	1
rel. err. (%)	4.58	1



Appendix D.2 - In-plane shear test - Load until failure

Comparison of the global responses: (predictions less accurate)

	Strength CPU Ti	
	[GPa]	[mins]
DNS	77.721	1435
VM	70.179	
rel. err. (%)	9.70	9
VM-Mod.	71.112	2
rel. err. (%)	8.50	
LVM	69.838	
rel. err. (%)	10.14	37
LVM-Mod.	70.747	57
rel. err. (%)	8.97	
VLM	69.155	0
rel. err. (%)	11.02	Э



Appendix D.1 - In-plane shear test - Load-Unload

Comparison of the global responses: (predictions less accurate)

	Strength [GPa]	CPU Time [mins]
DNS	76.906	1149
VM	70.048	
rel. err. (%)	8.92	0.2
VM-Mod.	70.865	0.2
rel. err. (%)	7.85	
LVM	69.677	
rel. err. (%)	9.40	4
LVM-Mod.	70.472	4
rel. err. (%)	8.37	
VLM	69.004	0
rel. err. (%)	10.27	2

