

Artificial Intelligence accelerated multi-scale simulations of Composite Material Failure

L. Noels, L. Wu, C. Anglade

Computational & Multiscale Mechanics of Materials – CM3

<http://www.ltas-cm3.ulg.ac.be/>

Allée de la découverte 9, B4000 Liège

L.Noels@ulg.ac.be

This project has received funding from the European Union's Horizon Europe Framework Programme under grant agreement No. 101056682 for the project "Digital DEsign strategies to certify and mAnufacture Robust cOmposite sTructures (DIDEAROT)". The contents of this publication are the sole responsibility of ULiege and do not necessarily reflect the opinion of the European Union. Neither the European Union nor the granting authority can be held responsible for them

This research has been funded by the Walloon Region under the agreement no. 2010092-CARBOBRAKE in the context of the M-ERA.Net Join Call 2020 funded by the European Union under the Grant Agreement no. 958174.

- 2-Scale problem

- Idea:

- Substitute the explicit constitutive model

$$\sigma_M(X, t) = \sigma_M(\varepsilon_M(X, t); \mathbf{z}_M(X, \tau), \tau \in [0, t])$$

- By an implicit relation resulting from the lower-scale BVP resolution

- Macro-scale state variables correspond to the set of RVE state variables

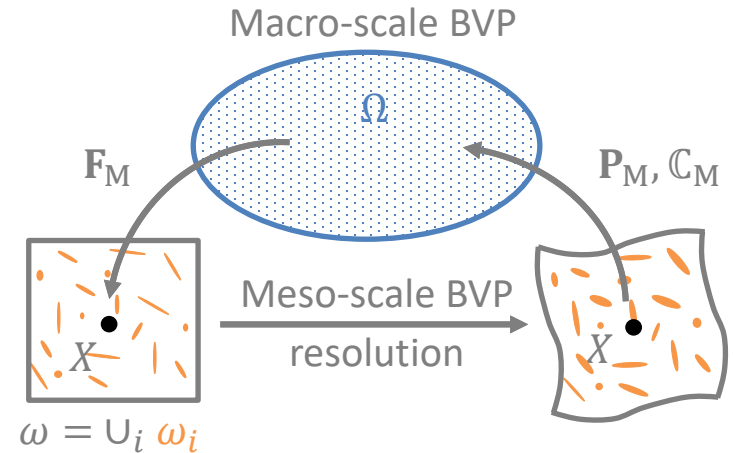
$$\mathbf{z}_M(X, t) = \{\mathbf{z}_m(\mathbf{x}, t) \forall \mathbf{x} \in \omega(X)\}$$

- Basic assumption: separation of scale

$$l_M \gg l_{RVE} \gg l_m$$

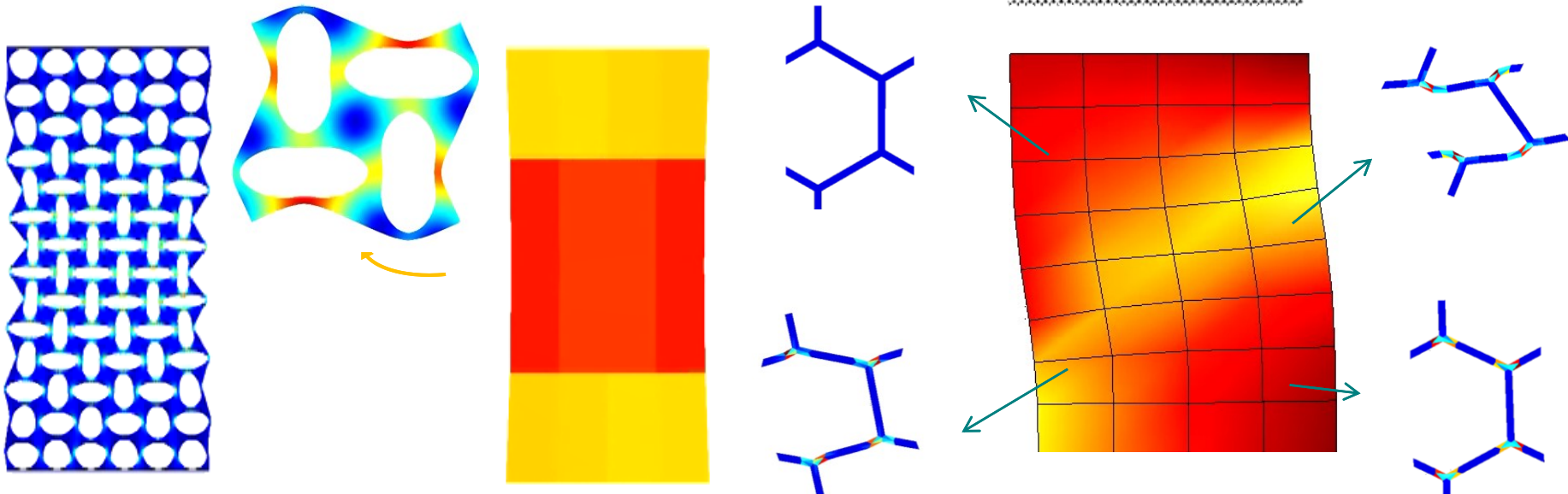
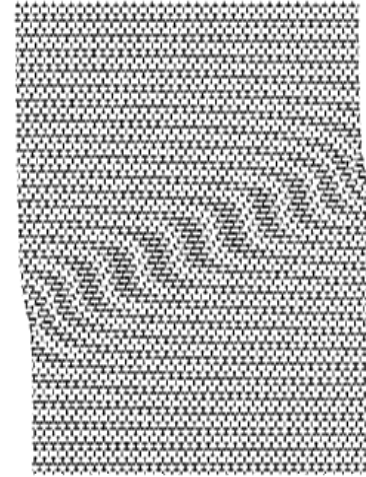
- Opportunities

- Complex simulations (accounting for complex failure modes)
- Stochastic analyses
- ...



- Multi-Scale FE² resolution
 - Method has been applied to a wide variety of problems
 - Several drawbacks
 - Overwhelming computation time
 - Fixed micro-structure

➔ Not manageable for real applications

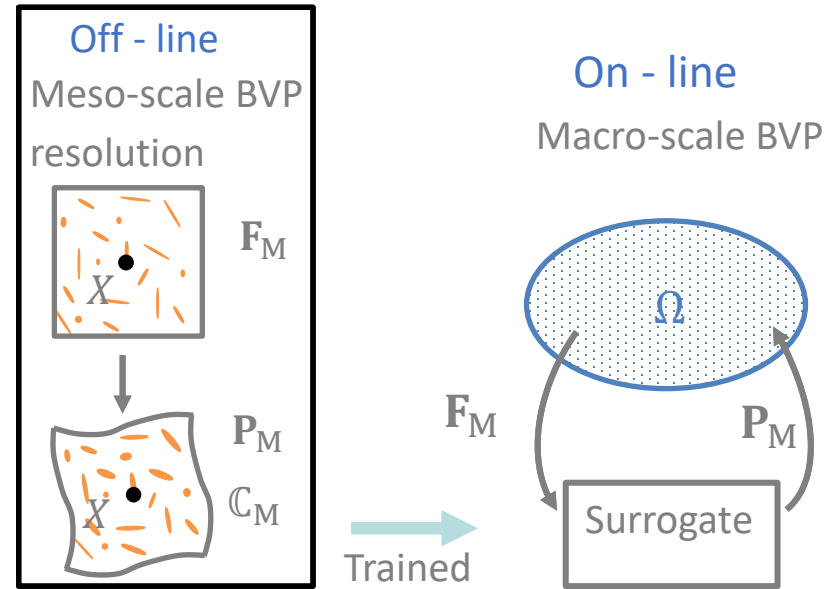


- Opportunities

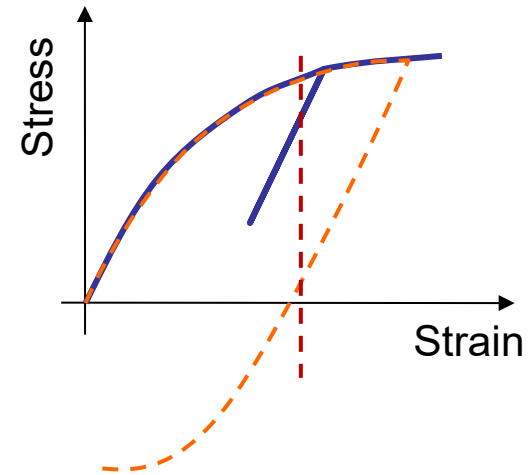
- Account for micro-structural effects on macro-scale responses
 - Failure origin
 - Micro-structural variation
- Accelerate simulations
 - Makes virtual testing possible

- Challenges

- Which surrogate/ML tool?
- How to get a relevant database?
- Quid extrapolating capabilities?

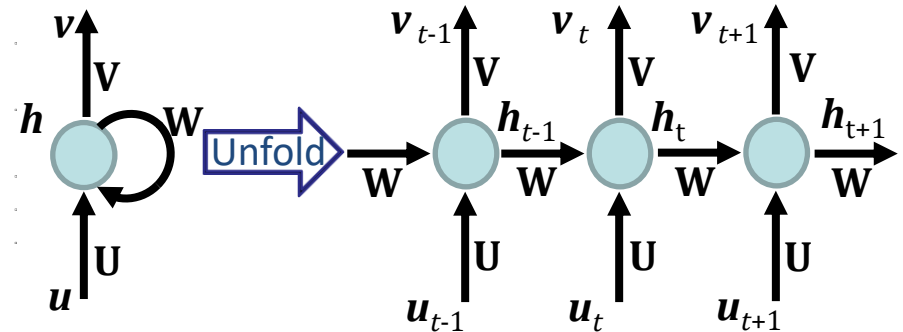
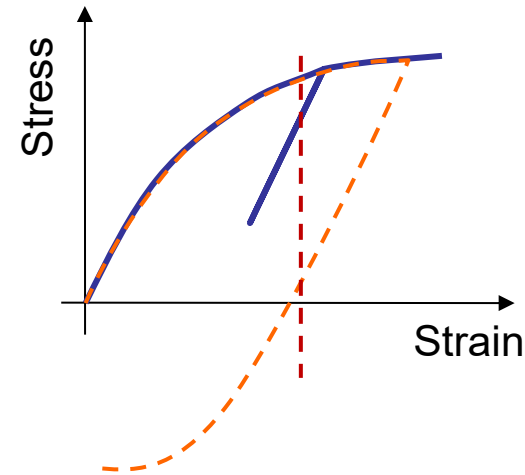


- Input / output definition
 - Input: Strain (history): $\mathbf{F}_M$
 - Output: Stress (history): $\mathbf{P}_M$
- Elasto-plastic material behaviour
 - No bijective strain-stress relation
 - Feed-forward NNW cannot be used
 - History should be accounted for



Recurrent Neural Network for multi-scale simulations

- Input / output definition
 - Input: Strain (history): $\mathbf{F}_M$
 - Output: Stress (history): $\mathbf{P}_M$
- Elasto-plastic material behaviour
 - No bijective strain-stress relation
 - Feed-forward NNW cannot be used
 - History should be accounted for
- Recurrent neural network
 - Allows a history dependent relation
 - Input: sequence $\mathbf{u}_t$
 - Output: sequence $\mathbf{v}_t = \mathbf{g}(\mathbf{u}_t, \mathbf{h}_{t-1})$
 - Internal variable $\mathbf{h}_t = \mathbf{g}(\mathbf{u}_t, \mathbf{h}_{t-1})$
 - Existing recurrent units
 - GRU, LSTM
 - Both developed for Nature Language Processing
 - ...

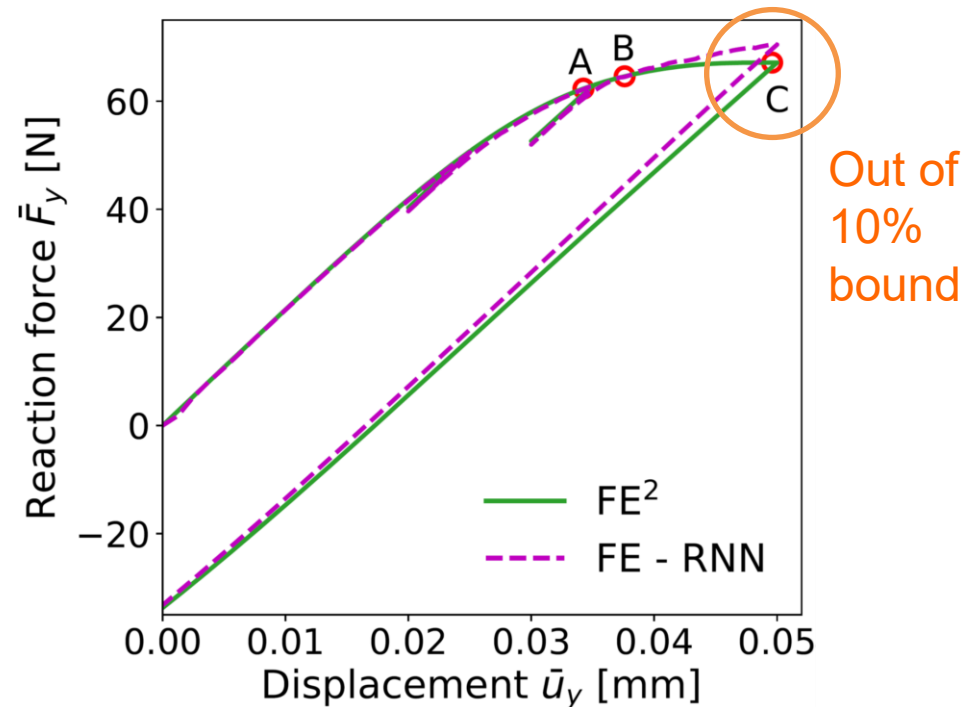
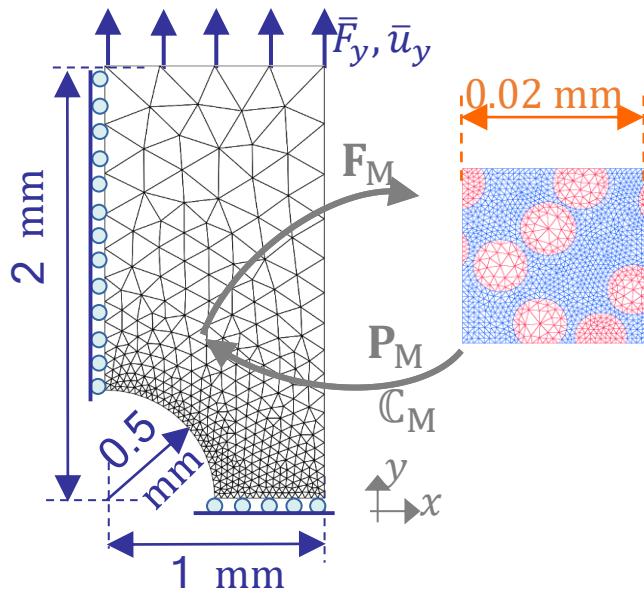


Recurrent Neural Network-accelerated multi-scale simulations

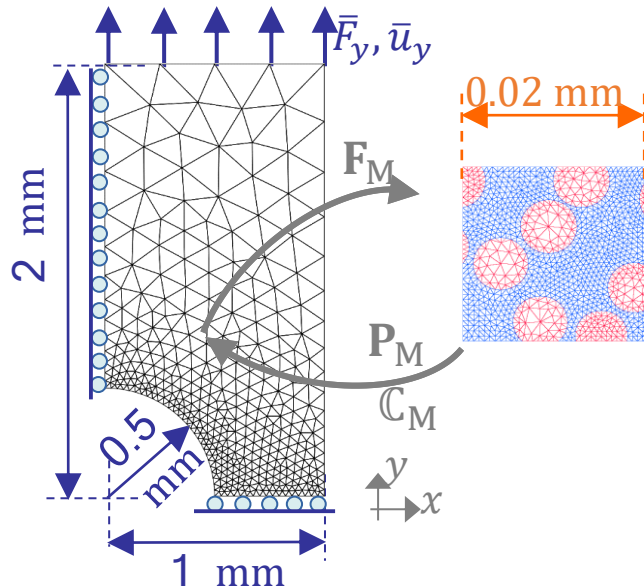
Multiscale simulation

- Use of a GRU as RNN
- Elasto-plastic composite RVE
- Comparison FE^2 vs. RNN-surrogate
- Training data
 - Bounded at 10% deformation

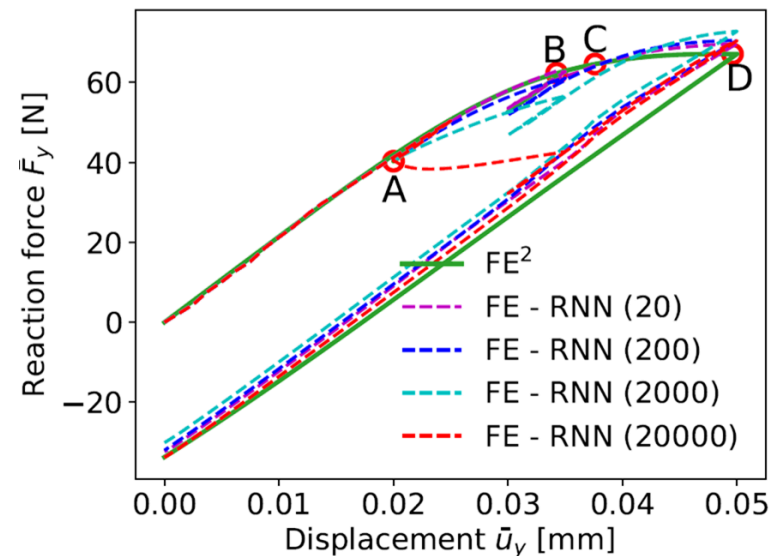
Off-line	FE^2	FE-RNN
Data generation	-	9000 x 2 h-cpu
Training	-	3 day-cpu
On-line	FE^2	FE-RNN
Simulation	18000 h-cpu	0.5 h-cpu



- What if online simulations use smaller increments?
 - Oscillations / loss of accuracy can appear with GRU, LSTM*
 - Both developed for Nature Language Processing
 - One needs to enforce self-consistency*
 - Need to replace the GRU/LSTM unit



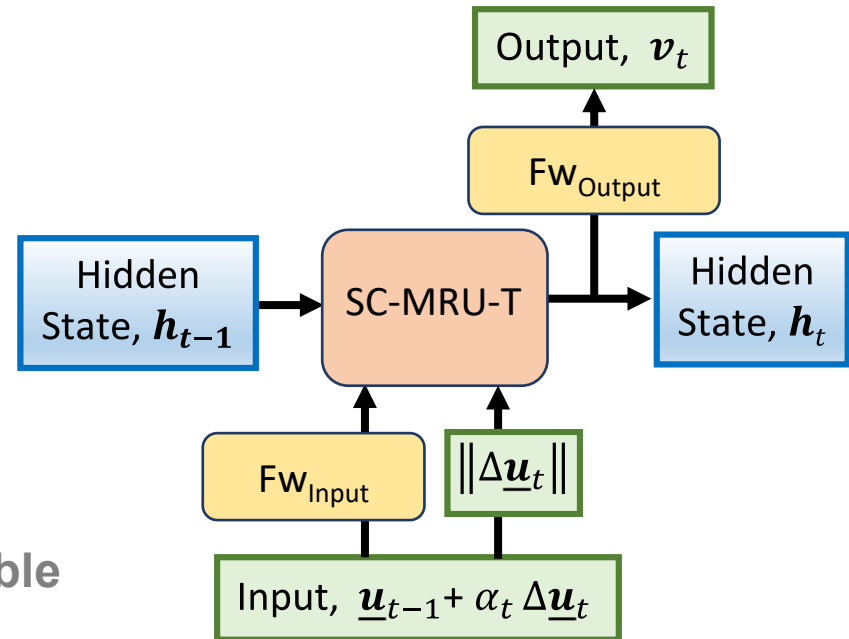
Simplified minimal recurrent unit



*Colin Bonatti, Dirk Mohr, On the importance of self-consistency in recurrent neural network models representing elasto-plastic solids, Journal of the Mechanics and Physics of Solids, 158, 2022, 104697, <https://doi.org/10.1016/j.jmps.2021.104697>.

Self-Consistent Recurrent Neural Network for multi-scale simulations

- The Self-Consistent Recurrent Neural Network based on a SC unit
 - Oscillations / loss of accuracy can appear with GRU, LSTM* -> SC required

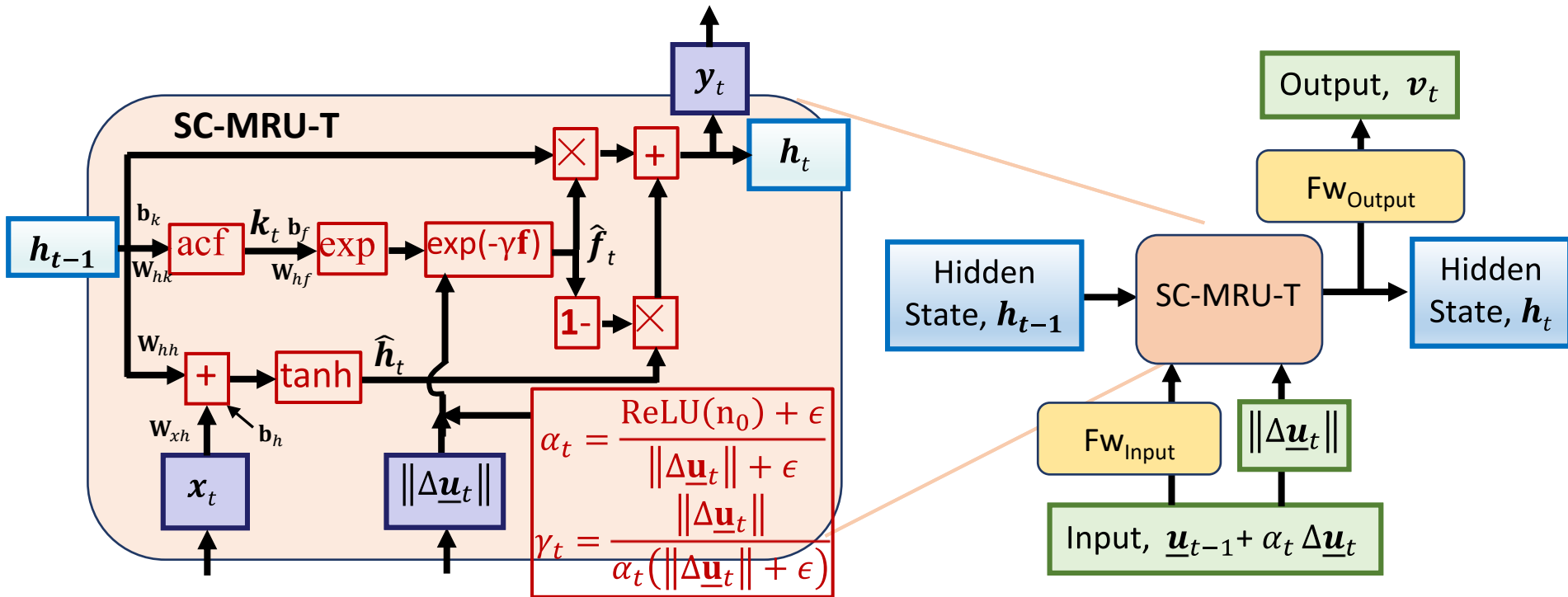


- The **total form of the input variable**
 - Use as input $\underline{u}_{t-1} + \alpha_t \Delta \underline{u}_t$
 - Lift the size of the input to the one of the hidden state with Fw_{input}
- & **increment norm** $\|\Delta \underline{u}_t\|$
 - For $\|\Delta \underline{u}_t\| \rightarrow 0$ the hidden state should not be updated
 - For larger $\|\Delta \underline{u}_t\|$, the hidden state should be updated

*Colin Bonatti, Dirk Mohr, On the importance of self-consistency in recurrent neural network models representing elasto-plastic solids, Journal of the Mechanics and Physics of Solids, 158, 2022, 104697, <https://doi.org/10.1016/j.jmps.2021.104697>.

Self-Consistent Recurrent Neural Network for multi-scale simulations

- The Developed Self-Consistent Minimal Recurrent Unit

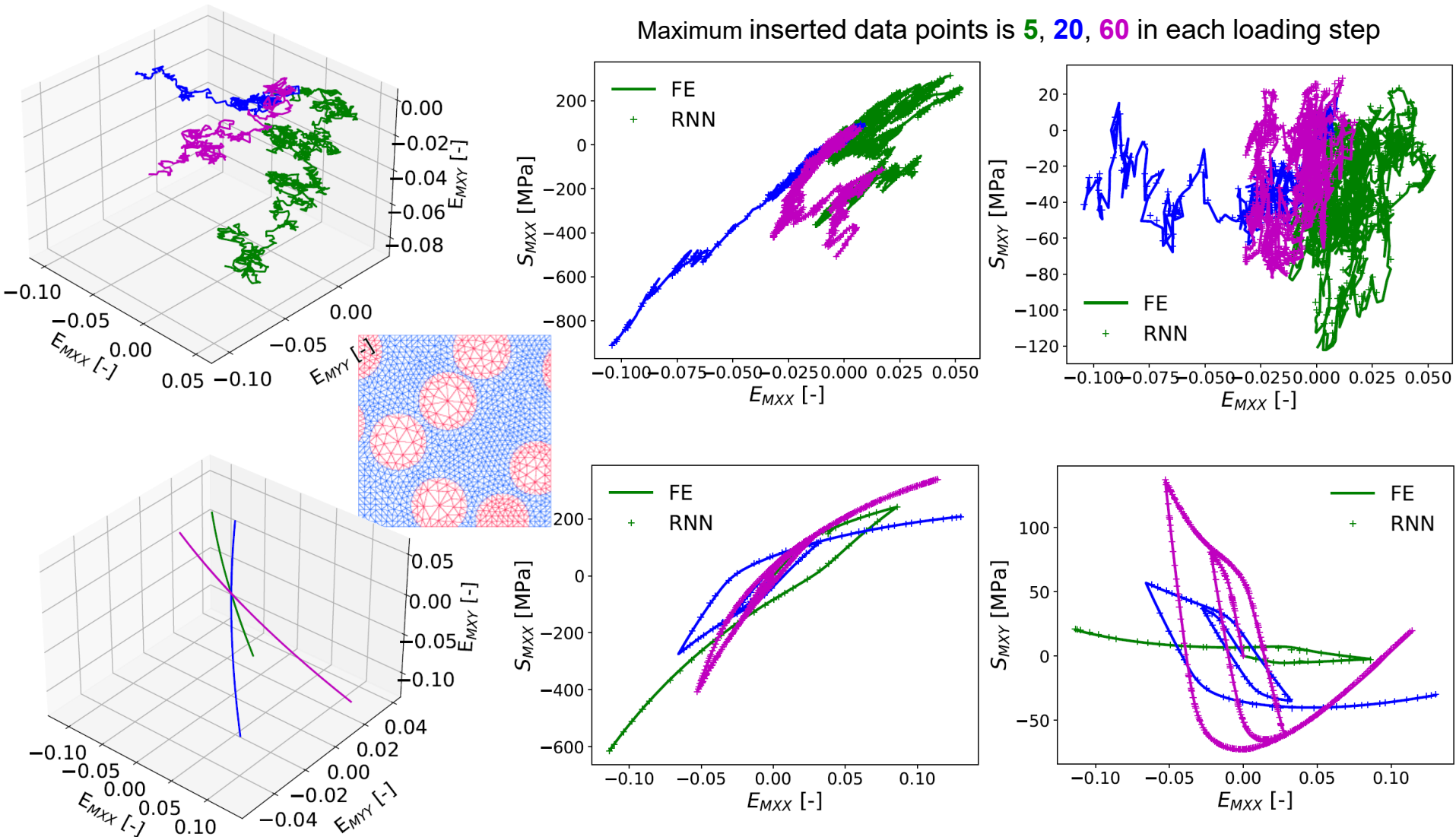


– Self-consistency enforced

- Double exponential function $f_t = \exp[w_f k_t + b_f] > 0$ & $\hat{f}_t = \exp[-\gamma(\|\Delta \underline{u}_t\|) f_t] \in [0, 1]$
- h_t is an element-wise interpolation (ratio $\hat{f}_t$ dependent on $\|\Delta \underline{u}_t\|$) between
 - previous value h_{t-1}
 - & update hidden variables $\hat{h}_t$
- n_0 is a learnable parameter

Self-Consistent Recurrent Neural Network for multi-scale simulations

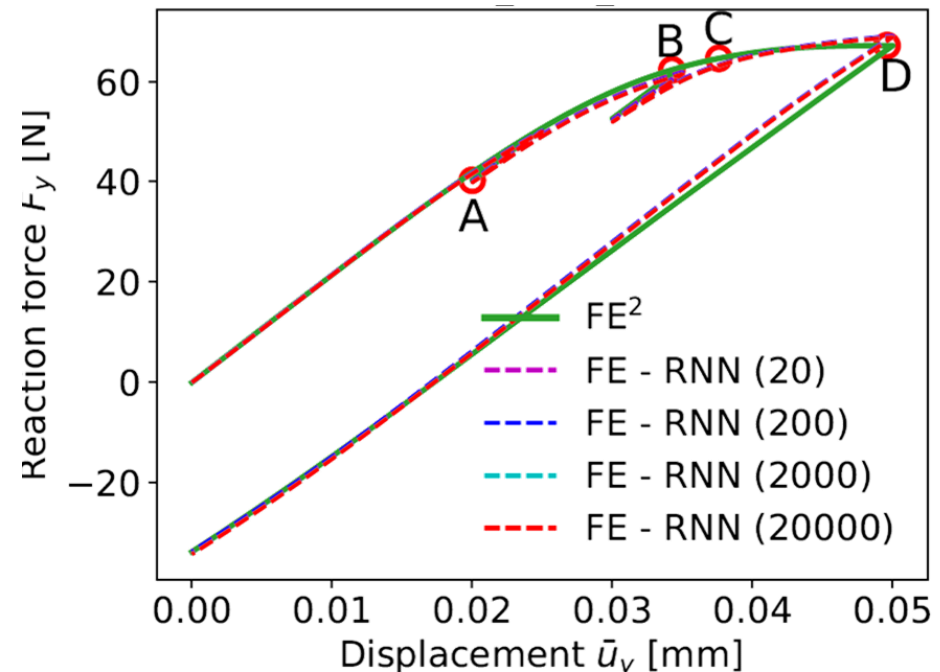
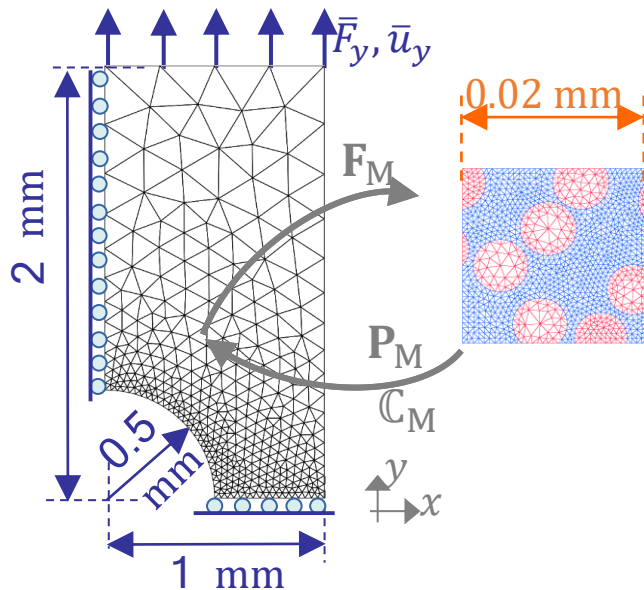
- SC-MRU-T: Testing data with inserted extra-points



Self-Consistent Recurrent Neural Network for multi-scale simulations

- FE2 vs. FE-RNN:
 - Change in the increment size between points A&B
 - Training is much faster with the SC-MRU cell

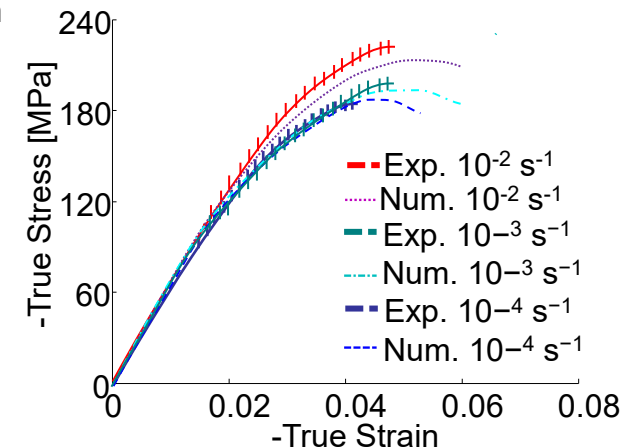
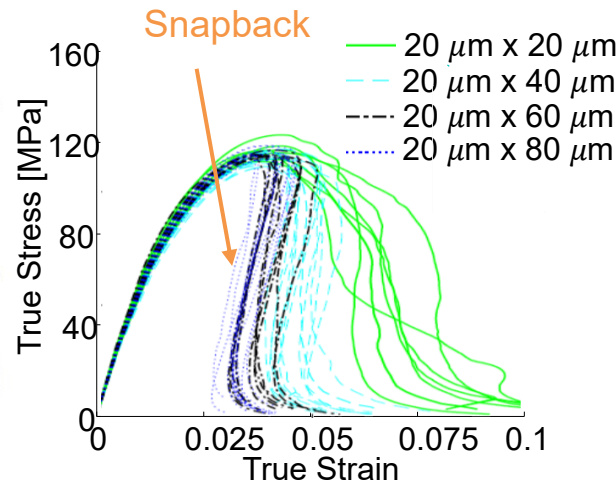
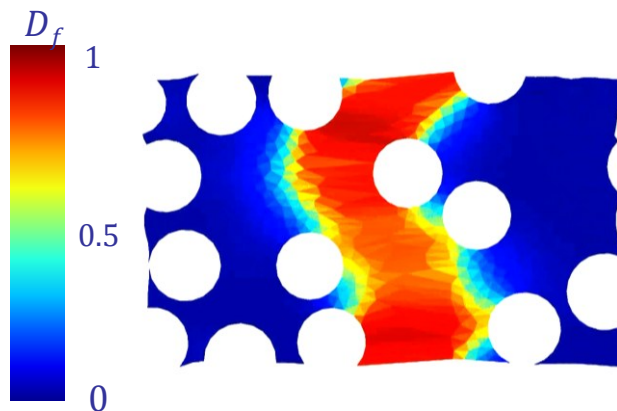
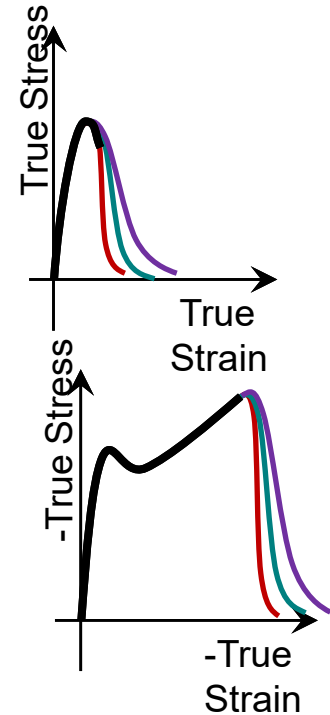
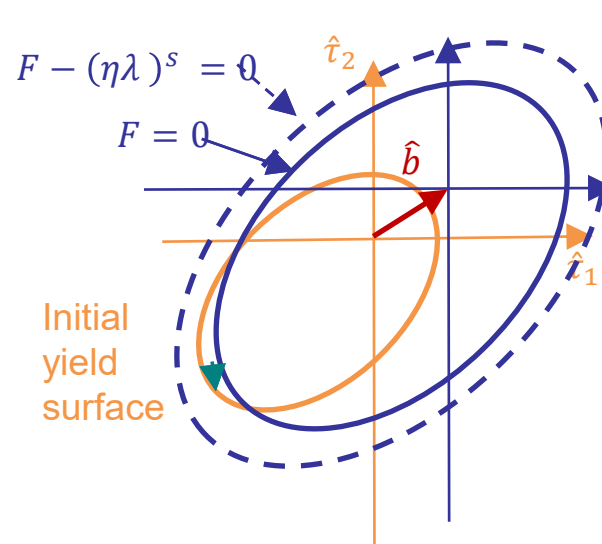
Off-line	FE ²	FE-GRU	FE-SC
Data generation	-	9000 x 2 h-cpu	23 500 h-cpu
Training	-	3 day-cpu	<10 h-cpu
On-line	FE ²	FE-GRU	FE-SC
Simulation	18000 h-cpu	0.5 h-cpu	0.4 h-cpu



AI-accelerated multi-scale analysis of composite failure

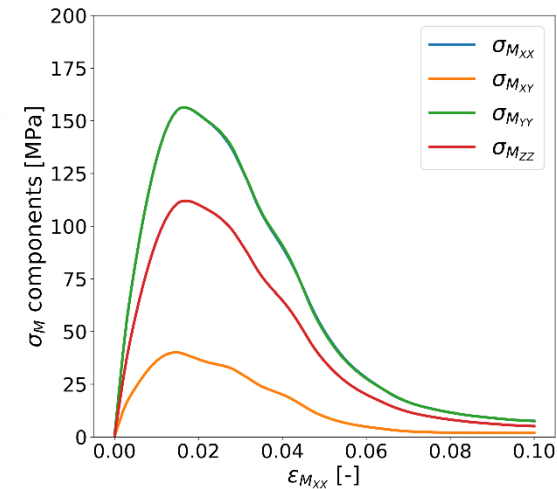
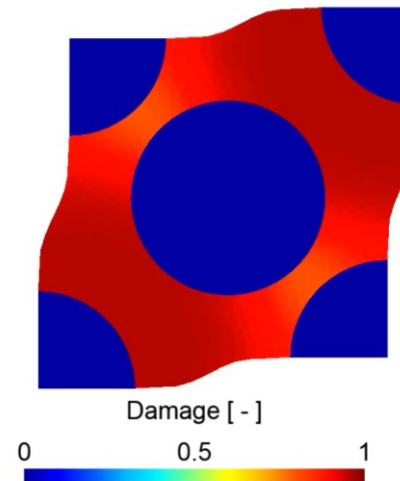
- RVE simulations:

- Complex material model for resin
 - (Visco-Elasticity-)Visco-plasticity with pressure dependency
 - Triaxiality-dependent damage models
 - Non-local damage models
- Transverse anisotropy for fibre
 - Failure with phase-field
- Experimentally validated



- Challenges to develop the AI surrogate:

- We need an extensive data-base
 - Simulations should reach total failure
 - Resin is brittle $\rightarrow$ snapback
- $\rightarrow$ (R)VE size is reduced



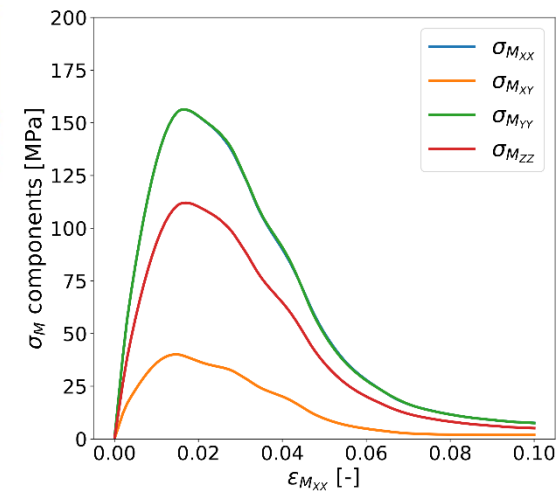
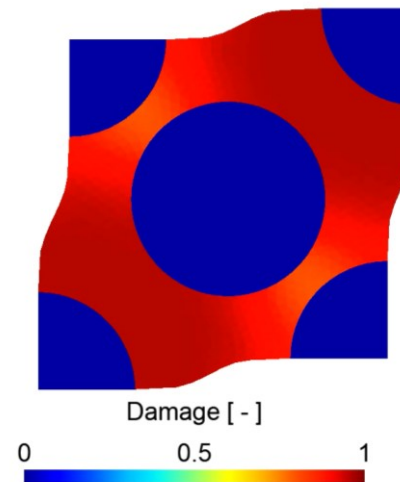
AI-accelerated multi-scale analysis of composite failure

- Challenges to develop the AI surrogate:

- We need an extensive data-base

- Simulations should reach total failure
- Resin is brittle → snapback

→ (R)VE size is reduced



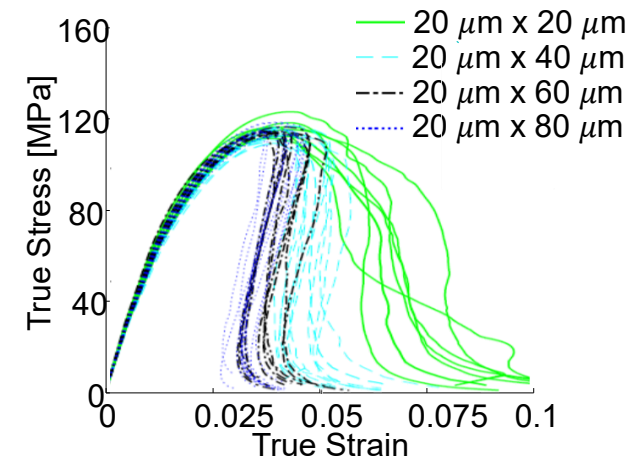
- Homogenized curves are meaningless

- They exhibit a strain softening
- Softening depends on the RVE size
- Only physical value is fracture energy G_c

→ We need to regularize the homogenized response

$$\tilde{\alpha} - l_c^2 \nabla^2 \tilde{\alpha} = \alpha$$

→ Parameter tuned to recover the fracture energy G_c



- Development of an embedding non-local framework:

- Identification of local/non-local variables

- Plastic strain tensor (from unloading in apparent space)

$$\boldsymbol{\varepsilon}_M^{\text{plast}} = \boldsymbol{\varepsilon}_M - \mathbb{C}_M^{\text{el},D^{-1}} : \boldsymbol{\sigma}_M$$

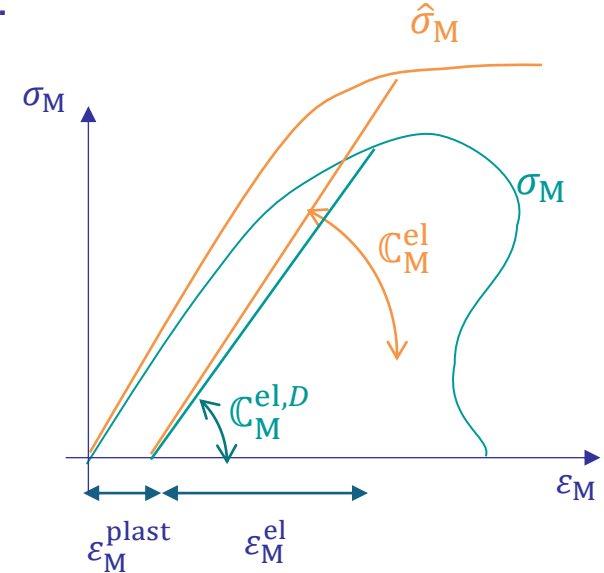
- Component-wise damage (to be reduced*)

$$D_{M_{ijkl}} = 1 - \frac{C_{M_{ijkl}}^{\text{el},D}}{C_{M_{ijkl}}^{\text{el}}}$$

- New macro-scale Helmholtz equations

$$D_{M_a} - l_d^2 \nabla^2 \tilde{D}_{M_a} = D_{M_a}$$

$$\tilde{\varepsilon}_{M_b}^{\text{plast}} - l_p^2 \nabla^2 \tilde{\varepsilon}_{M_b}^{\text{plast}} = \varepsilon_{M_b}^{\text{plast}}$$



*J. Yvonnet, Q-C. He, P. Li, Reducing internal variables and improving efficiency in data-driven modelling of anisotropic damage from RVE simulations, Computational Mechanics 72 (2023), p 37-55

- Development of an embedding non-local framework:

- Identification of local/non-local variables

- Plastic strain tensor (from unloading in apparent space)

$$\boldsymbol{\varepsilon}_M^{\text{plast}} = \boldsymbol{\varepsilon}_M - \mathbb{C}_M^{\text{el},D^{-1}} : \boldsymbol{\sigma}_M$$

- Component-wise damage (to be reduced*)

$$D_{M_{ijkl}} = 1 - \frac{C_{M_{ijkl}}^{\text{el},D}}{C_{M_{ijkl}}^{\text{el}}}$$

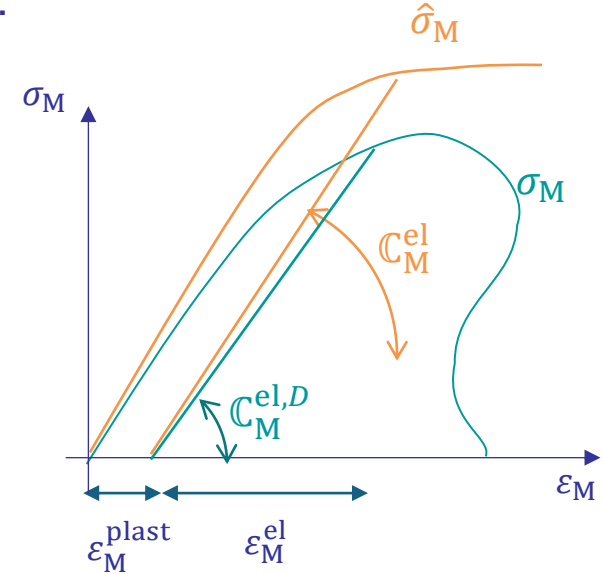
- New macro-scale Helmholtz equations

$$D_{M_a} - l_d^2 \nabla^2 \tilde{D}_{M_a} = D_{M_a}$$

$$\tilde{\varepsilon}_{M_b}^{\text{plast}} - l_p^2 \nabla^2 \tilde{\varepsilon}_{M_b}^{\text{plast}} = \varepsilon_{M_b}^{\text{plast}}$$

- Reconstructed (mesh-insensitive) apparent stress

$$\boldsymbol{\sigma}_{M_{\text{rec}}} = [(1 - \tilde{D}_M) \odot \mathbb{C}_M^{\text{el}}] : (\boldsymbol{\varepsilon}_M - \tilde{\boldsymbol{\varepsilon}}_M^{\text{plast}})$$



- Development of an embedding non-local framework:

- Identification of local/non-local variables

- Plastic strain tensor (from unloading in apparent space)

$$\boldsymbol{\varepsilon}_M^{\text{plast}} = \boldsymbol{\varepsilon}_M - \mathbb{C}_M^{\text{el},D^{-1}} : \boldsymbol{\sigma}_M$$

- Component-wise damage (to be reduced*)

$$D_{M_{ijkl}} = 1 - \frac{C_{M_{ijkl}}^{\text{el},D}}{C_{M_{ijkl}}^{\text{el}}}$$

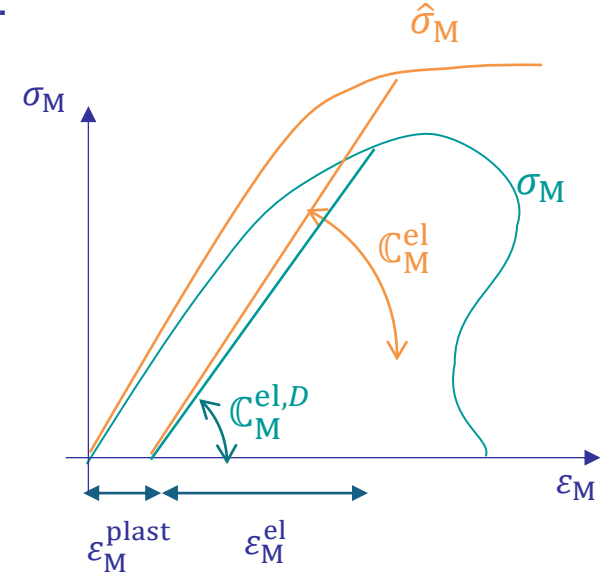
- New macro-scale Helmholtz equations

$$D_{M_a} - l_d^2 \nabla^2 \tilde{D}_{M_a} = D_{M_a}$$

$$\tilde{\varepsilon}_{M_b}^{\text{plast}} - l_p^2 \nabla^2 \tilde{\varepsilon}_{M_b}^{\text{plast}} = \varepsilon_{M_b}^{\text{plast}}$$

- Reconstructed (mesh-insensitive) apparent stress

$$\boldsymbol{\sigma}_{M_{\text{rec}}} = [(1 - \tilde{D}_M) \odot \mathbb{C}_M^{\text{el}}] : (\boldsymbol{\varepsilon}_M - \tilde{\boldsymbol{\varepsilon}}_M^{\text{plast}})$$



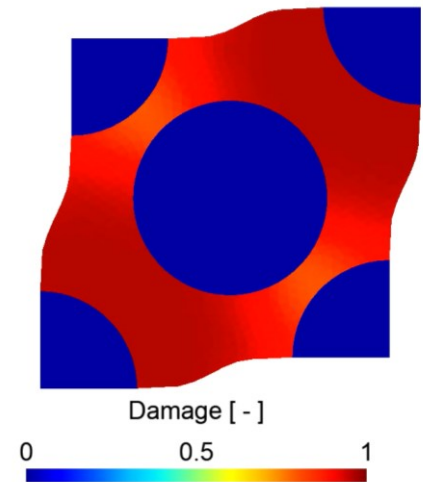
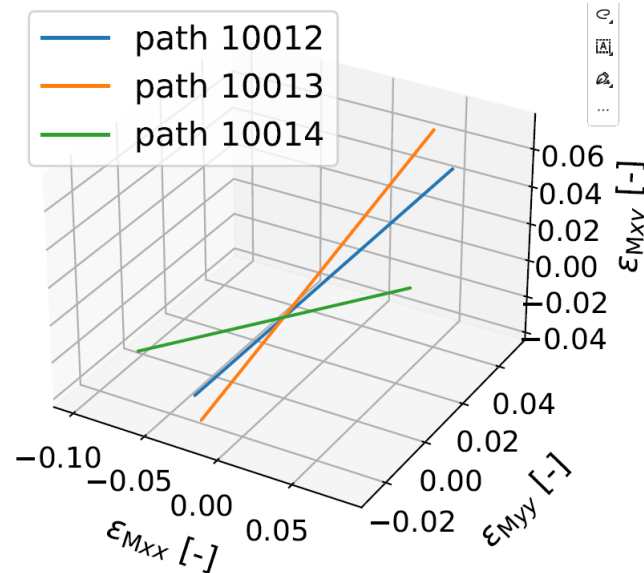
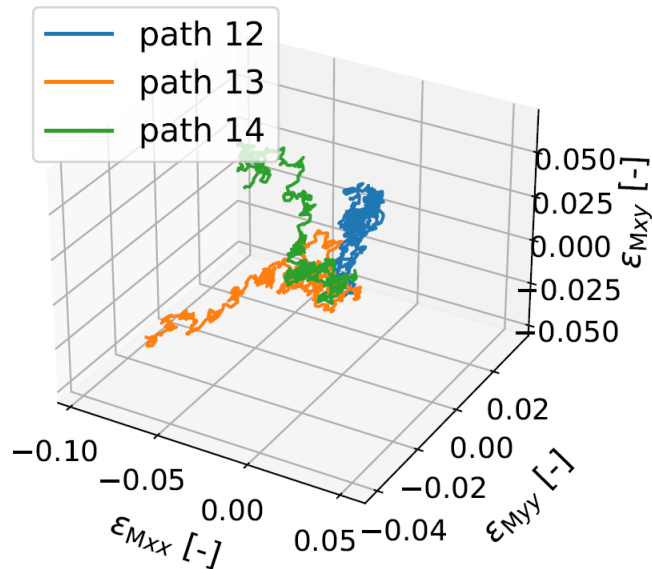
➡ Neural networks to be developed:

- Inputs: $\underline{\mathbf{u}}_t = \{\boldsymbol{\varepsilon}_M\}_t$
- Outputs: $\underline{\mathbf{v}}_t = \{\boldsymbol{\sigma}_M, \mathbb{C}_M^{\text{el},D}, \mathbb{C}_M^{\text{el}}\}_t$

- Training data-base

- ~10 000 random paths

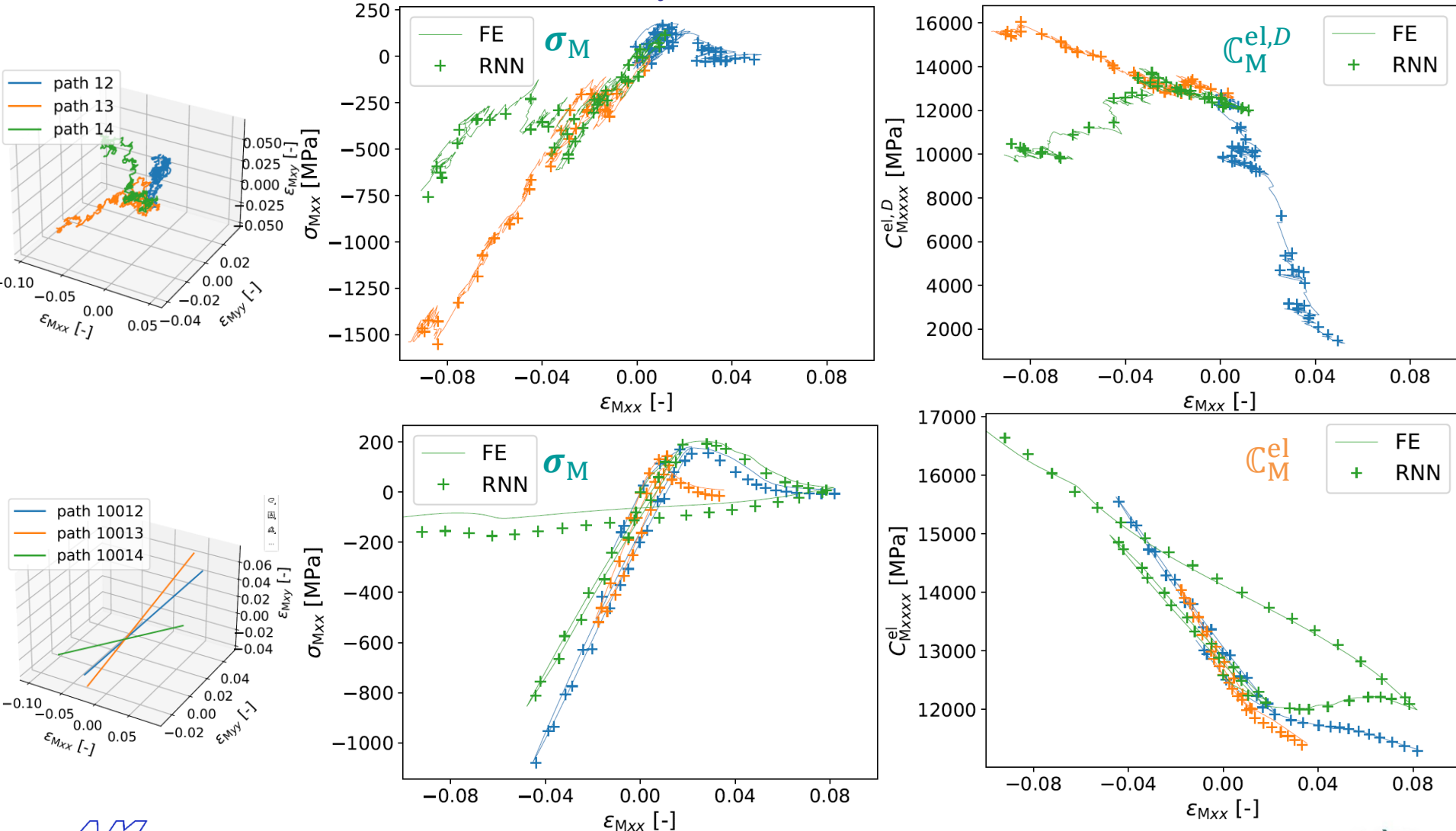
- ~ 5000 cyclic paths



AI-accelerated multi-scale analysis of composite failure

- Testing the neural networks

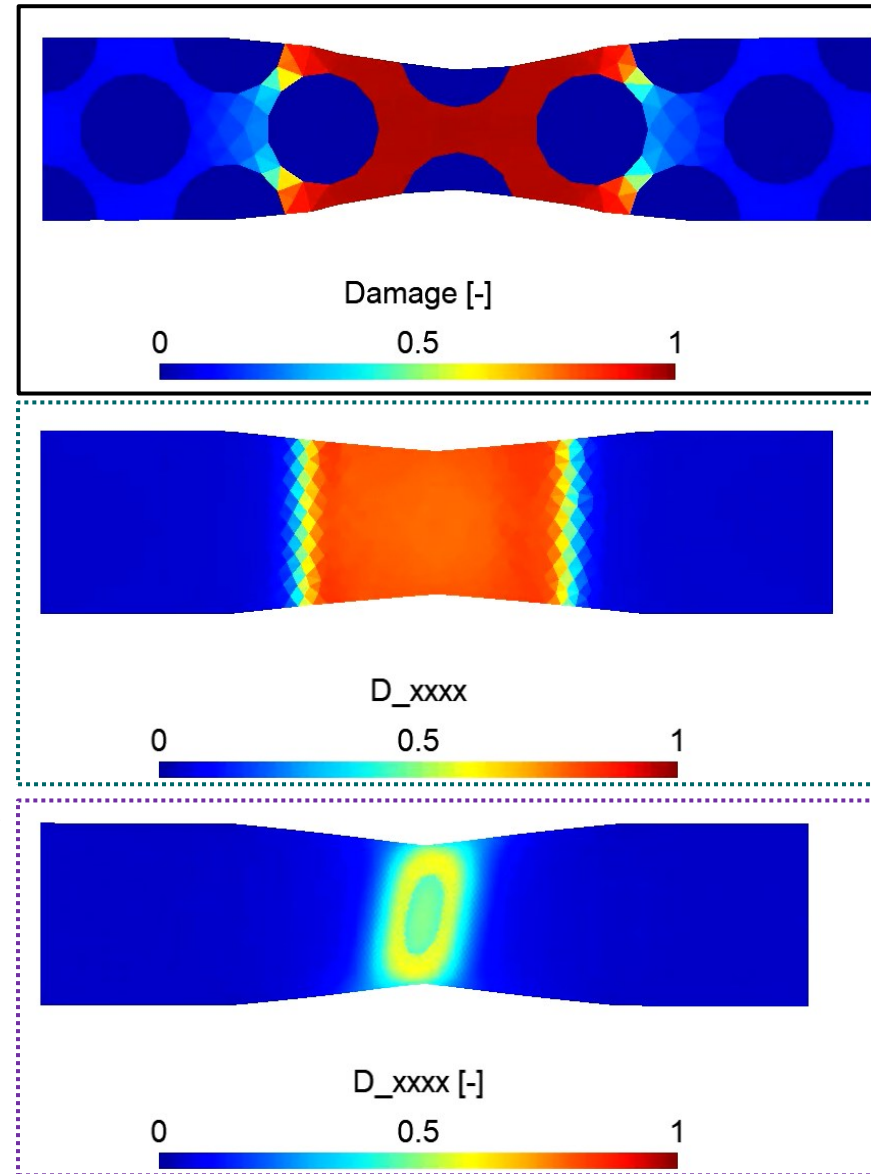
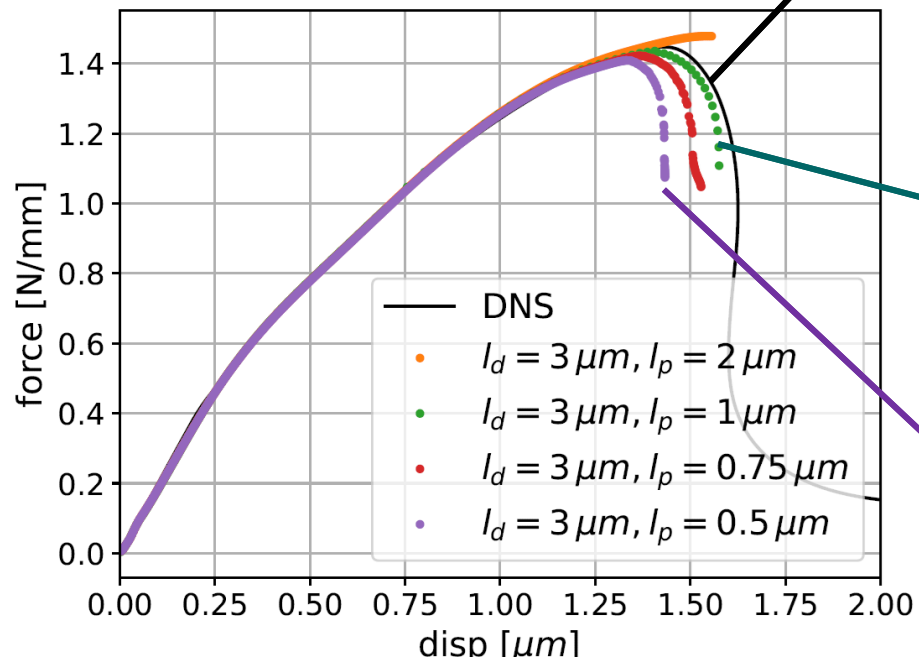
– $\underline{u}_t = \{\boldsymbol{\varepsilon}_M\}_t$ vs. $\underline{v}_t = \{\boldsymbol{\sigma}_M, \mathbb{C}_M^{\text{el},D}, \mathbb{C}_M^{\text{el}}\}_t$



- Non-local lengths

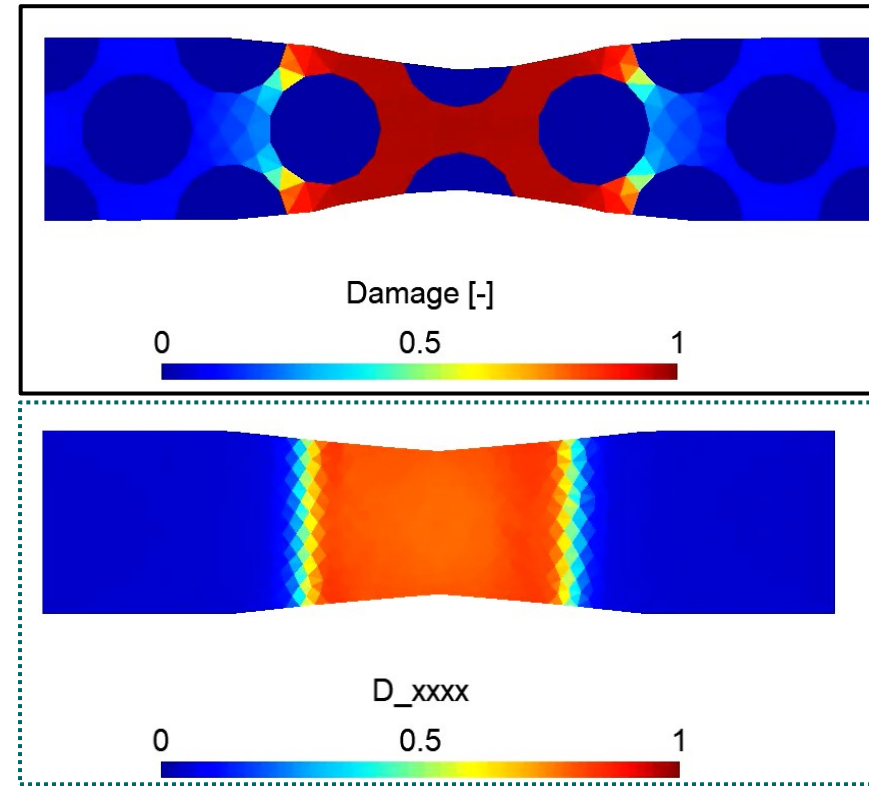
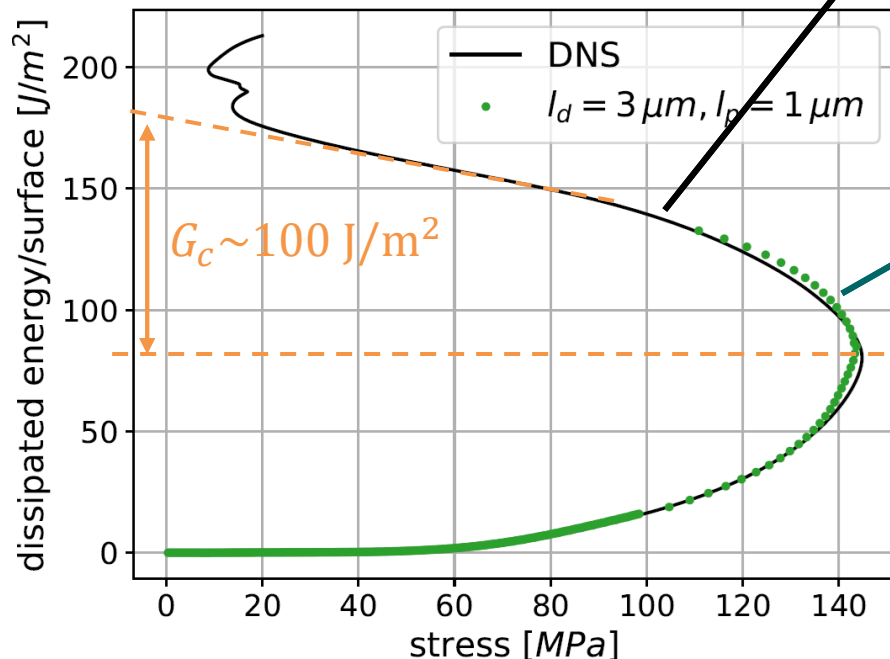
- $$\begin{cases} D_{M_a} - l_d^2 \nabla^2 \tilde{D}_{M_a} = D_{M_a} \\ \tilde{\varepsilon}_{M_b}^{\text{plast}} - l_p^2 \nabla^2 \tilde{\varepsilon}_{M_b}^{\text{plast}} = \varepsilon_{M_b}^{\text{plast}} \end{cases}$$

- Calibration from DNS

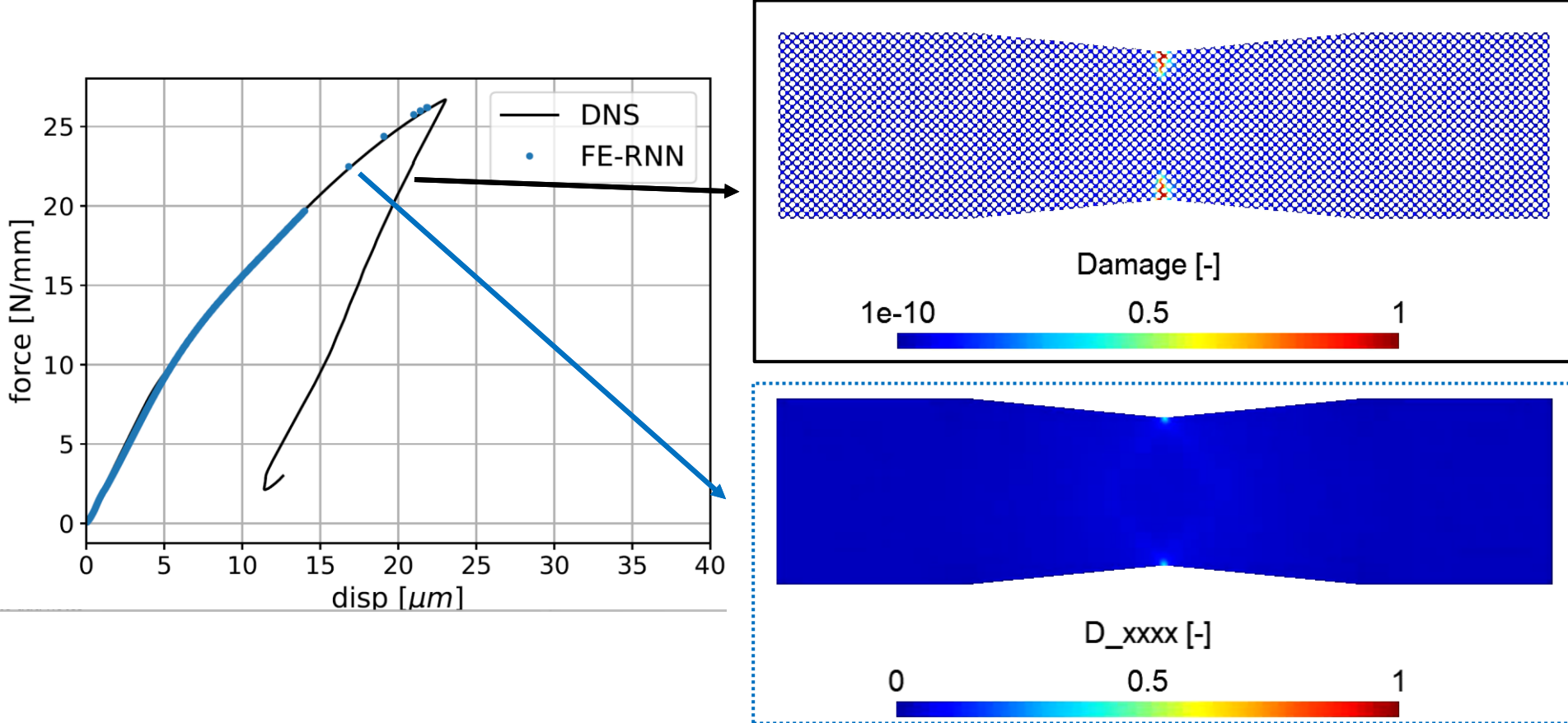


- Non-local lengths

- $$\begin{cases} D_{M_a} - l_d^2 \nabla^2 \tilde{D}_{M_a} = D_{M_a} \\ \tilde{\varepsilon}_{M_b}^{\text{plast}} - l_p^2 \nabla^2 \tilde{\varepsilon}_{M_b}^{\text{plast}} = \varepsilon_{M_b}^{\text{plast}} \end{cases}$$
- Calibration from DNS



- Larger sample
 - DNS vs. RNN
 - RNN trained on volume elements
 - Calibrated macro-scale non-local lengths



- Conclusions

- Data-driven method for failure analysis
- Need more rigorous damage definition

- Materials

- Open source code :
<http://www.ltas-cm3.ulg.ac.be/openSource.htm>
- Publications
<http://www.ltas-cm3.ulg.ac.be/publications.htm>
- Data: <http://www.ltas-cm3.ulg.ac.be/openSource.htm>



- Credits

- MOAMMM: This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862015 of the H2020-EU.1.2.1. - FET Open Programme
- DIDEAROT: This project has received funding from the European Union's Horizon Europe Framework Programme under grant agreement No. 101056682. The contents of this publication are the sole responsibility of ULiege and do not necessarily reflect the opinion of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

