

Damage multi-scale simulations with a machine learning based surrogate



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Computational & Multiscale
Mechanics of Materials –
CM3

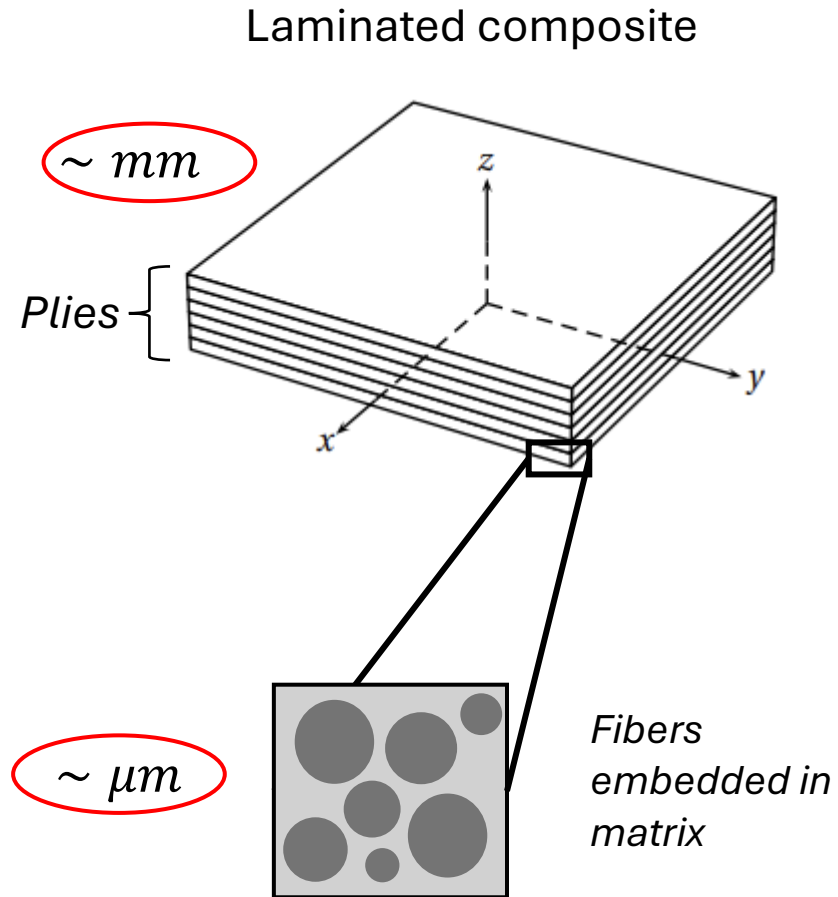
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Composites

A multiscale material



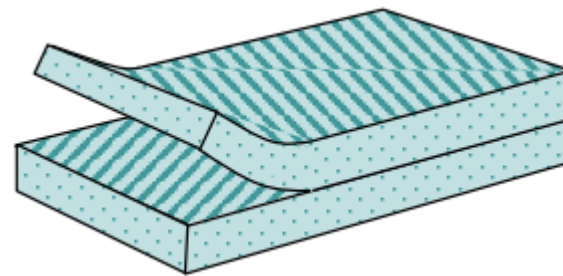
A complex failure

Brittle material

→ macroscopically: no plastic deformation

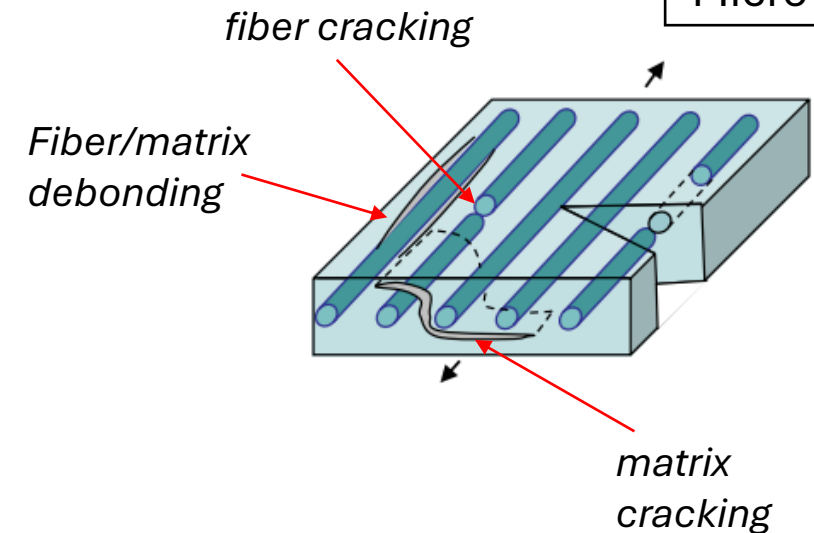
Different failure modes:

Macro



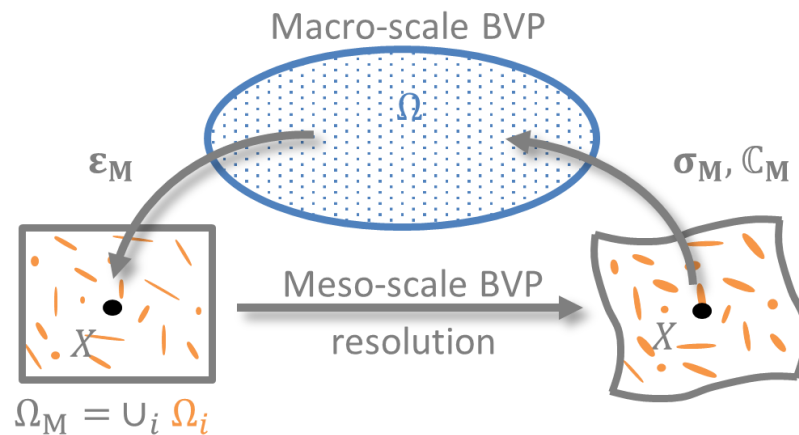
Delamination

Micro



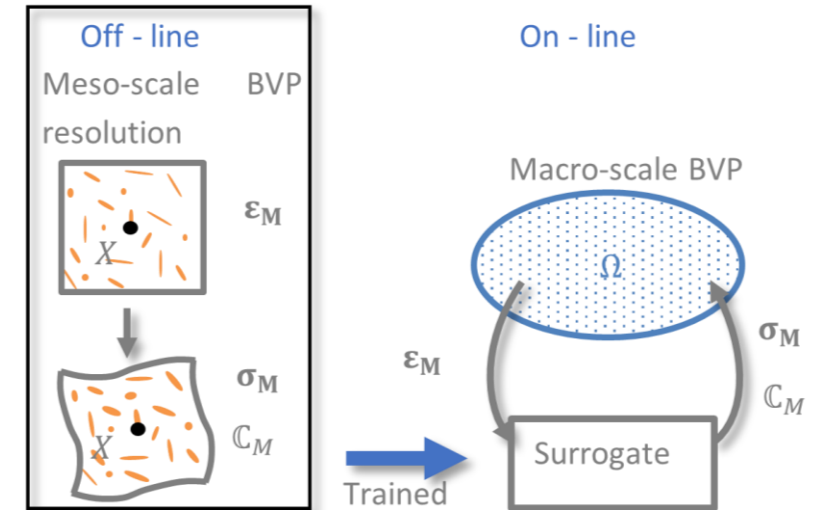
Multi-scale simulations

FE²



→ very high cost

Surrogate models



Training database: RVE simulations

→ speed-up of several orders

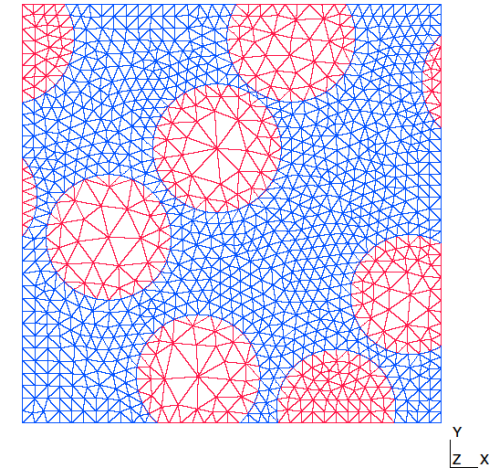
(**machine learning based
surrogates** particularly efficient)

Goal: surrogate-based multiscale model with damage

Challenges of surrogate-based multi-scale simulations with damage

- 1) Same challenges as continuous damage model (**CDM**) simulations in general
BUT with the difficulty to represent **internal variables at the homogenized level**

- 2) When using a **surrogate**,
 - it must be able to handle **history effects**
 - **no more access** to micro-scale internal variables

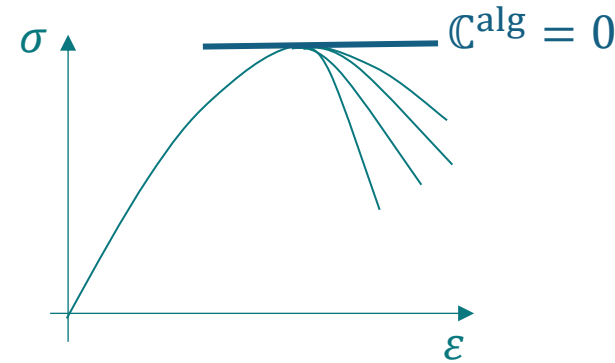


The challenge of CDM simulations in general

- I. *Non-local framework*
- II. *Surrogate (RNN)*
- III. *Multi-scale simulations*

Problems in simulations with damage:

- Loss of ellipticity
- Mesh dependency due to strain localisation



⇒ A solution: non-local equations

$$\tilde{\alpha} - l_c^2 \nabla^2 \tilde{\alpha} = \alpha \quad \left(\text{satisfies: } \int_{\Omega_0} \tilde{\alpha} \, dV = \int_{\Omega_0} \alpha \, dV \right)$$

Parameter tuned to recover the fracture energy G_c



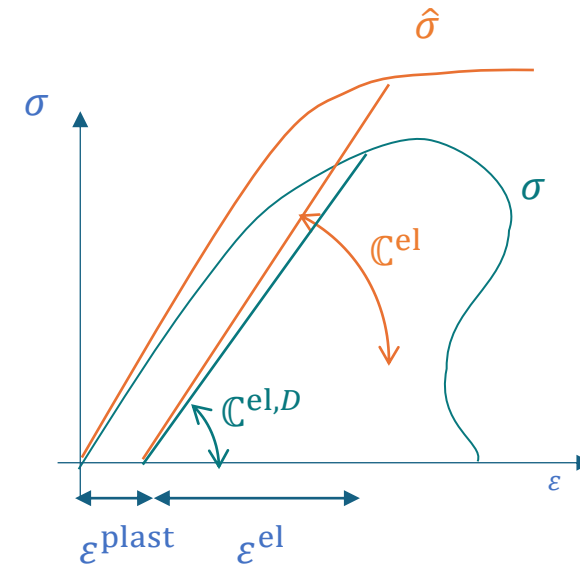
At macro-scale: need variables in non-local equations that we can define at the RVE level

The non-local formulation

- I. *Non-local framework*
- II. *Surrogate (RNN)*
- III. *Multi-scale simulations*

The non-local variables:

- The plastic strain: $\boldsymbol{\varepsilon}^{plast} = \boldsymbol{\varepsilon} - \mathbb{C}^{el,D^{-1}} : \boldsymbol{\sigma}$
(2nd order tensor)
- The damage: $D_{ijkl} = 1 - \frac{C_{ijkl}^{el,D}}{C_{ijkl}^{el}}$
(4th order tensor)



RVE behaviour

The reconstructed stress:

$$\begin{aligned}\boldsymbol{\sigma}_{rec} &= \mathbb{C}_{rec}^{el,D} : (\boldsymbol{\varepsilon} - \tilde{\boldsymbol{\varepsilon}}^{plast}) \\ &= [(\mathbb{U} - \tilde{\mathbb{D}}) \odot \mathbb{C}^{el}] : (\boldsymbol{\varepsilon} - \tilde{\boldsymbol{\varepsilon}}^{plast})\end{aligned}$$

The non-local formulation

- I. *Non-local framework*
- II. *Surrogate (RNN)*
- III. *Multi-scale simulations*

The system to be solved:

$$\begin{cases} \boldsymbol{\sigma}_{\text{rec}} \cdot \boldsymbol{\nabla} + \mathbf{b} = 0 \\ D_a - l_c^2 \nabla^2 \tilde{D}_a = D_a \\ \tilde{\varepsilon}_b^{\text{plast}} - l_c^2 \nabla^2 \tilde{\varepsilon}_b^{\text{plast}} = \varepsilon_b^{\text{plast}} \end{cases} \longrightarrow$$

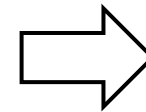
General,

The local law can be:

- A constitutive law
- A surrogate

The system size (27 at most):

- 21 independent variables for $\mathbb{D}$
(symmetries)
- 6 independent variables for $\boldsymbol{\varepsilon}^{\text{plast}}$
(symmetries)



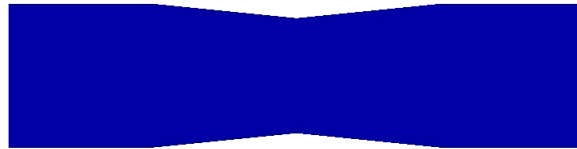
A reduction of the number of non-local variables could be desirable

Test with a constitutive law as a local law

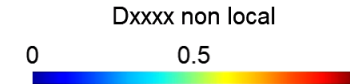
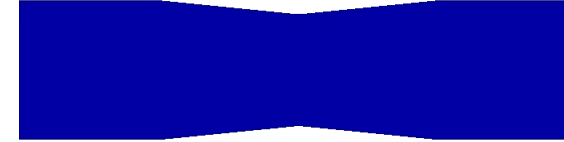
(testing the formulation here
→ the material is **not a composite**
→ **not a multiscale** simulation)

- I. *Non-local framework*
- II. *Surrogate (RNN)*
- III. *Multi-scale simulations*

(1)

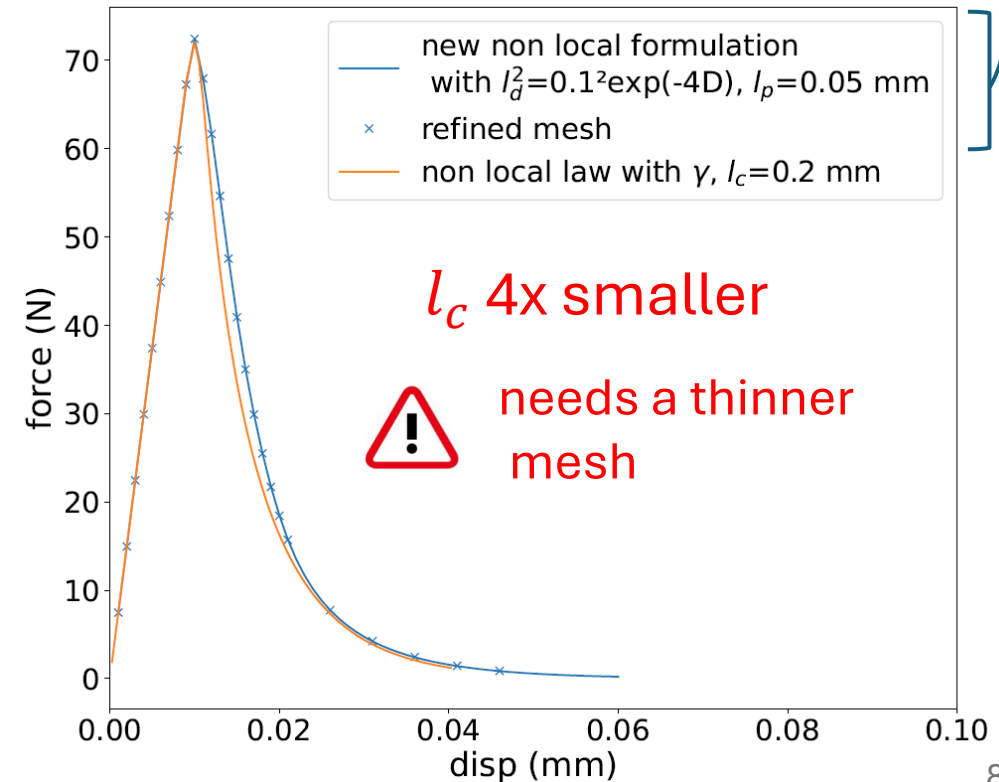
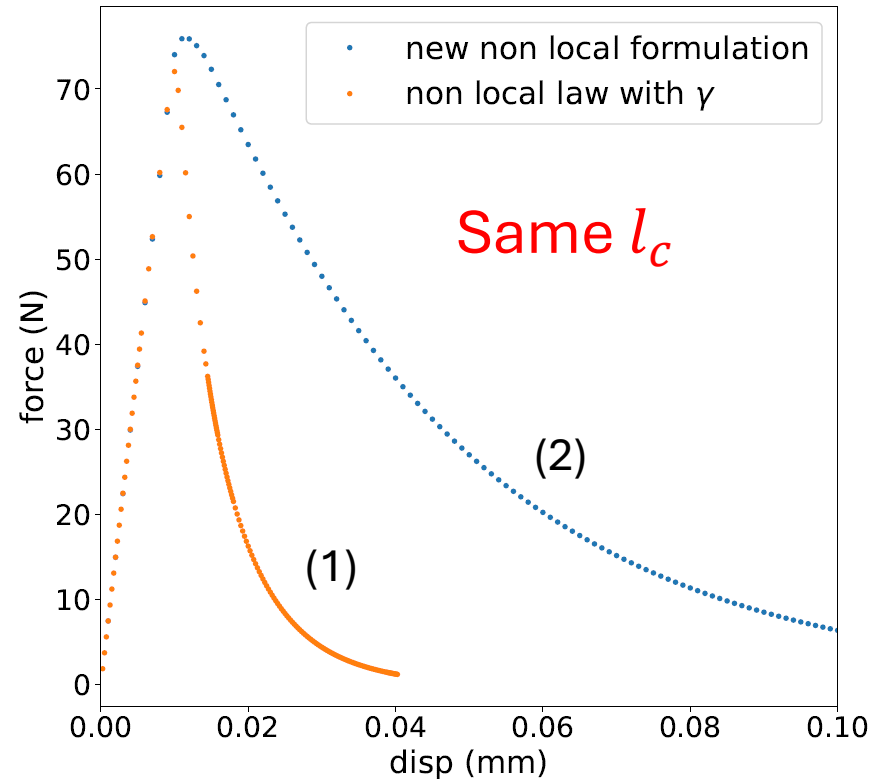


(2)



mesh insensitivity
recovered

Comparison with a
reference (true) non-
local formulation:



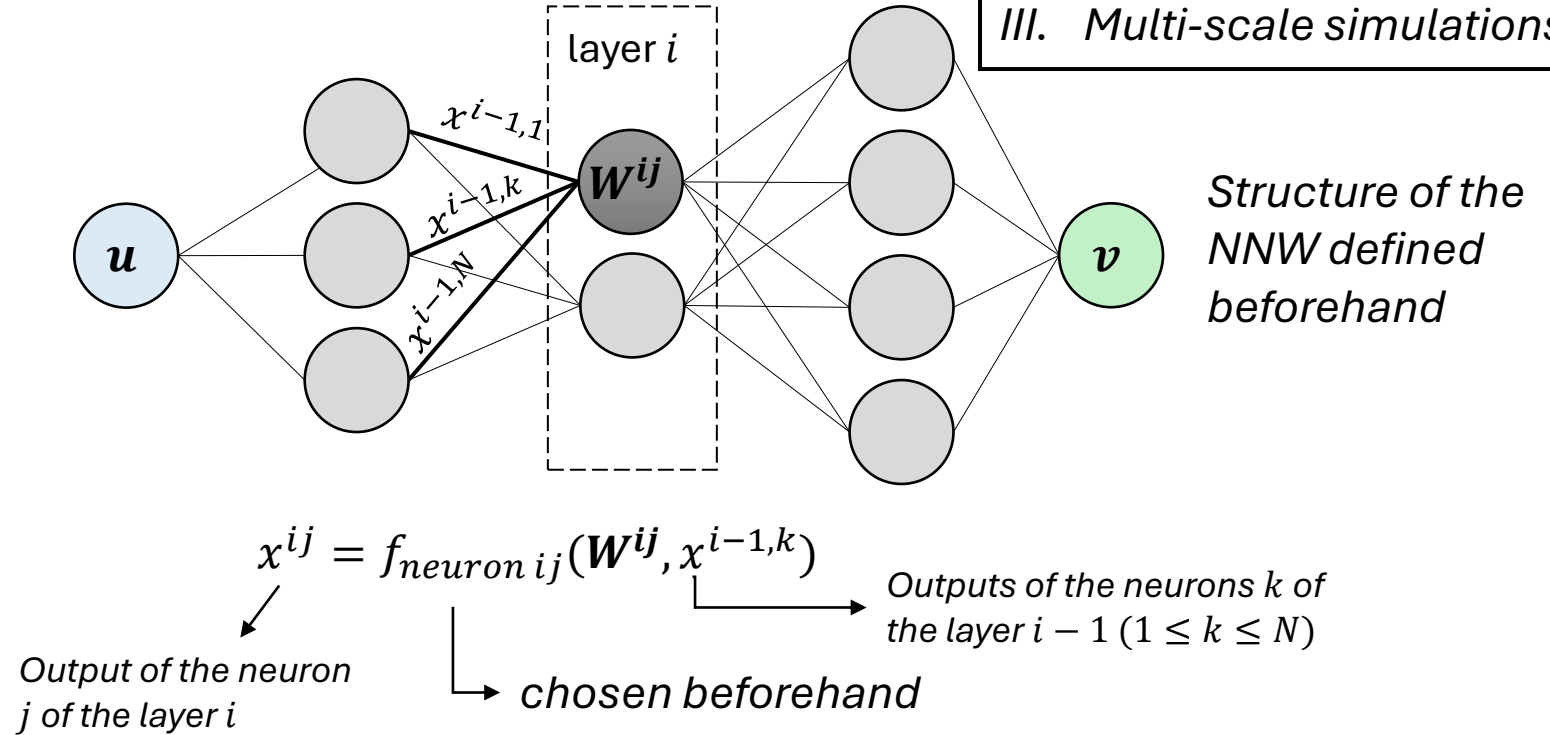
Neural Networks (NNW)

A NNW **models** the relation between a field u and a field v :

$$v = f_{NNW}(u)$$

$\downarrow$ output $\downarrow$ input

very complex function



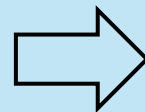
- I. Non-local framework
- II. **Surrogate (RNN)**
- III. Multi-scale simulations

How to obtain f_{NNW} ? $\rightarrow$ need to find the weights W^{ij}

Step 1: Collect a database

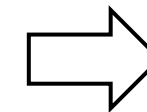
$$\{u_p, v_p\}_{1 \leq p \leq n}$$

find a way to obtain



Step 2: Training on the database

Find the best W^{ij} to have the **predictions** $f_{NNW}(u_p)$ **close to real** outputs v_p

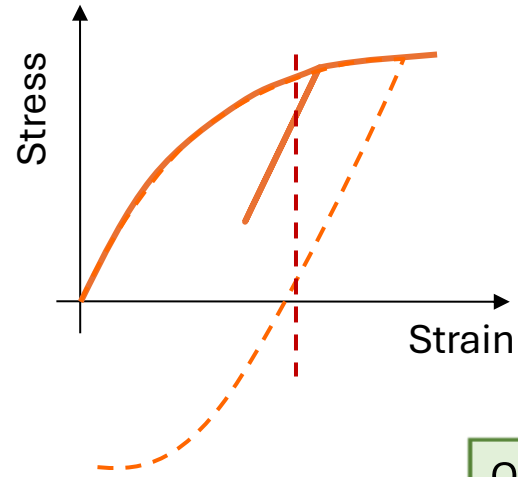


Step 3: Use the NNW

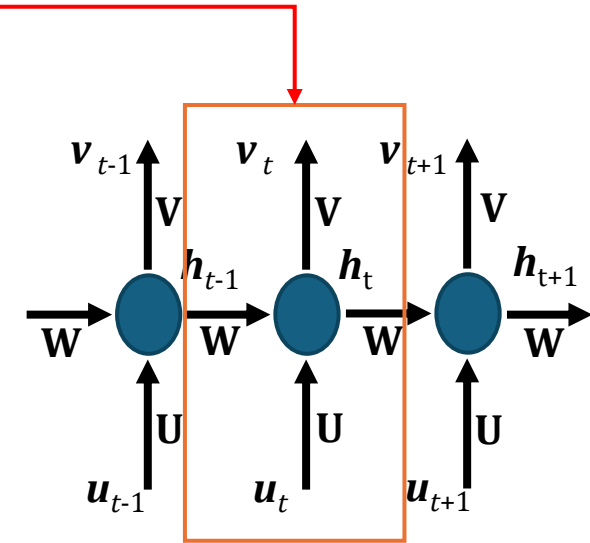
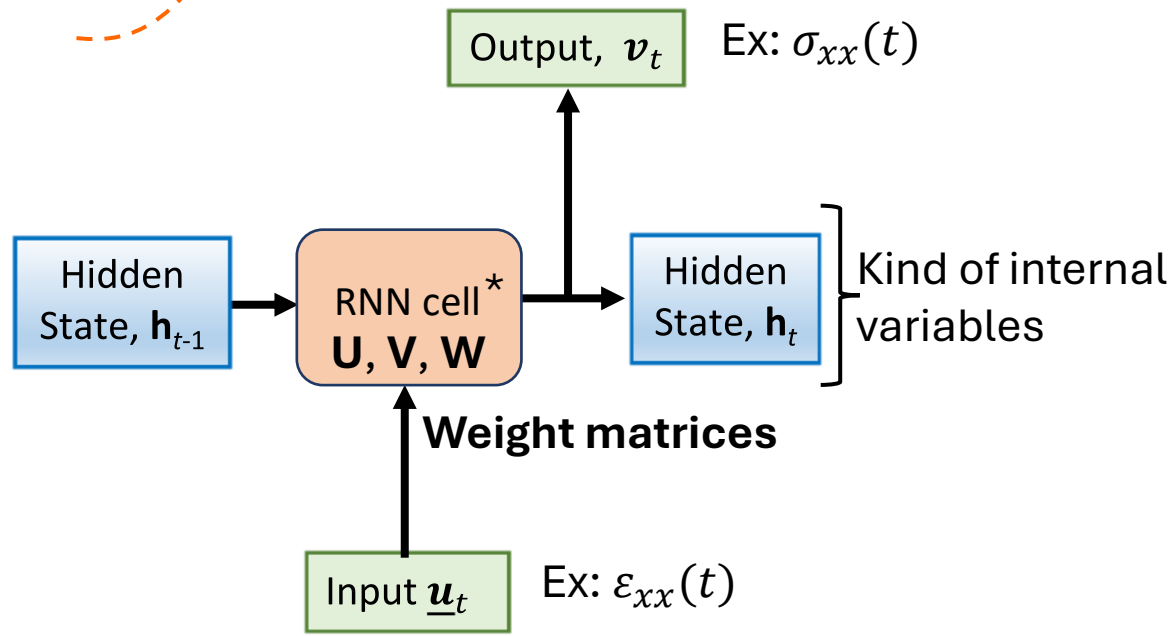
- f_{NNW} is defined
- New predictions $f_{NNW}(u_{new}) = v$

Recurrent Neural Network (RNN)

- I. Non-local framework
- II. **Surrogate (RNN)**
- III. Multi-scale simulations



Neural Network model for **history dependent relation**



Trained with sequences

$$\left[\begin{array}{c} \left\{ \mathbf{u}_{t-n}^{(p)} \right\} \\ \left\{ \mathbf{v}_{t-n}^{(p)} \right\} \end{array} , \dots , \begin{array}{c} \left\{ \mathbf{u}_t^{(p)} \right\} \\ \left\{ \mathbf{v}_t^{(p)} \right\} \end{array} \right]_{p=1, \dots, P}$$

* SC-MRU-T cell used
→ detailed in the next talk

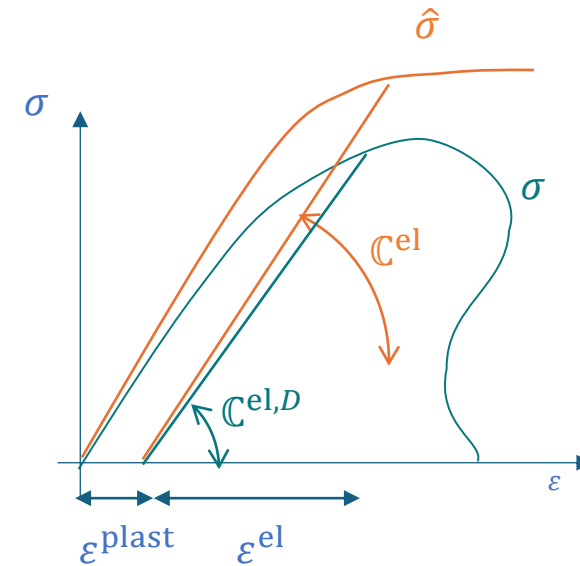
The inputs and outputs of the RNN

- I. Non-local framework
- II. **Surrogate (RNN)**
- III. Multi-scale simulations

The inputs: $\{\varepsilon_{M_{xx}}, \varepsilon_{M_{yy}}, \varepsilon_{M_{xy}}\}$

The outputs:

- The stresses: $\sigma_{M_{xx}}, \sigma_{M_{yy}}, \sigma_{M_{zz}}, \sigma_{M_{xy}}$
- The components $C_{M_{ijkl}}^{el,D}$
(elastic tangent with damage)
- The components $C_{M_{ijkl}}^{el}$
(elastic tangent without damage)



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

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

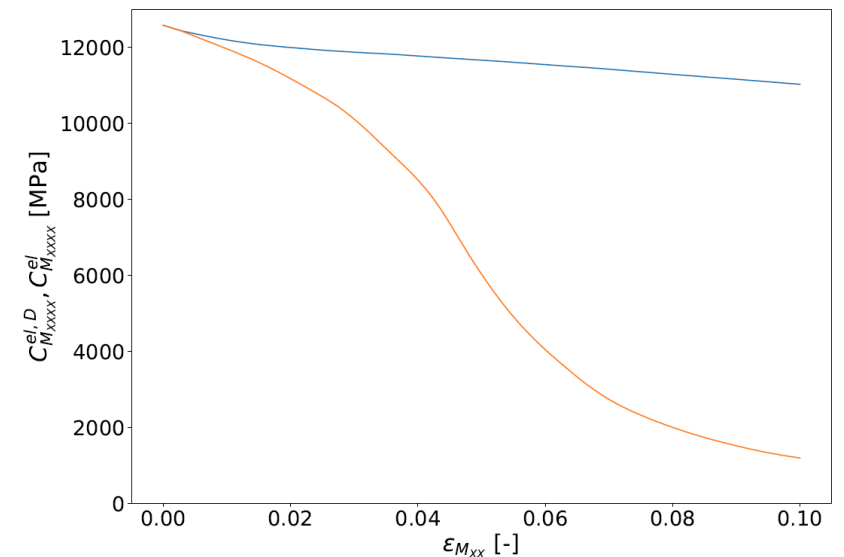
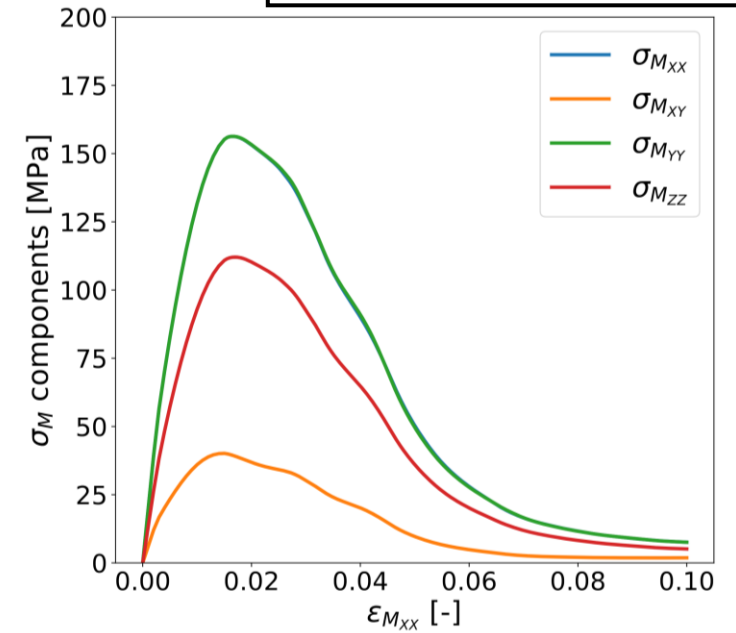
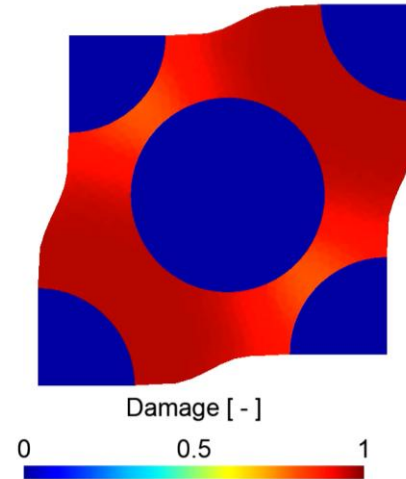
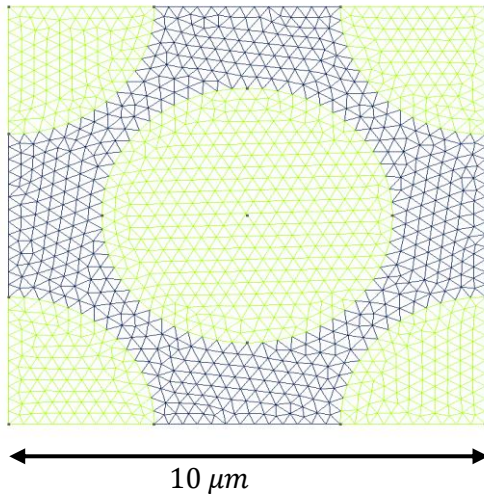
3 very different kinds of data

⇒ 3 RNN, one per output type

The RVE used as an application

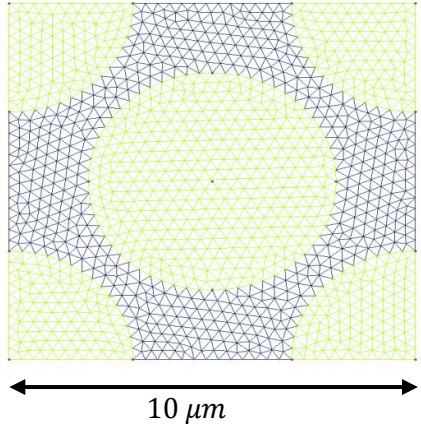
- I. Non-local framework
- II. **Surrogate (RNN)**
- III. Multi-scale simulations

RVE: a simple 2D periodic cell
60% fibre volume fraction

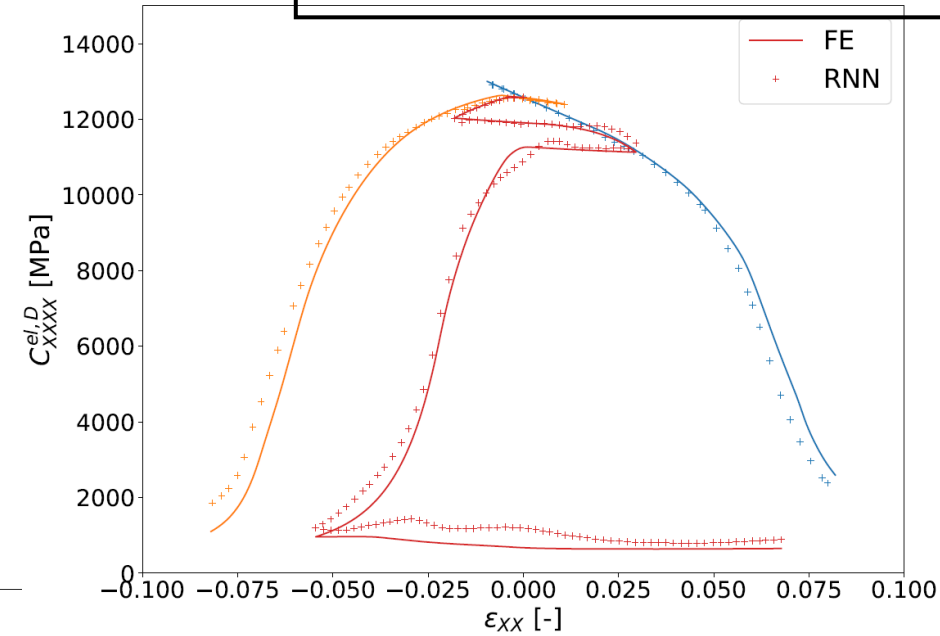
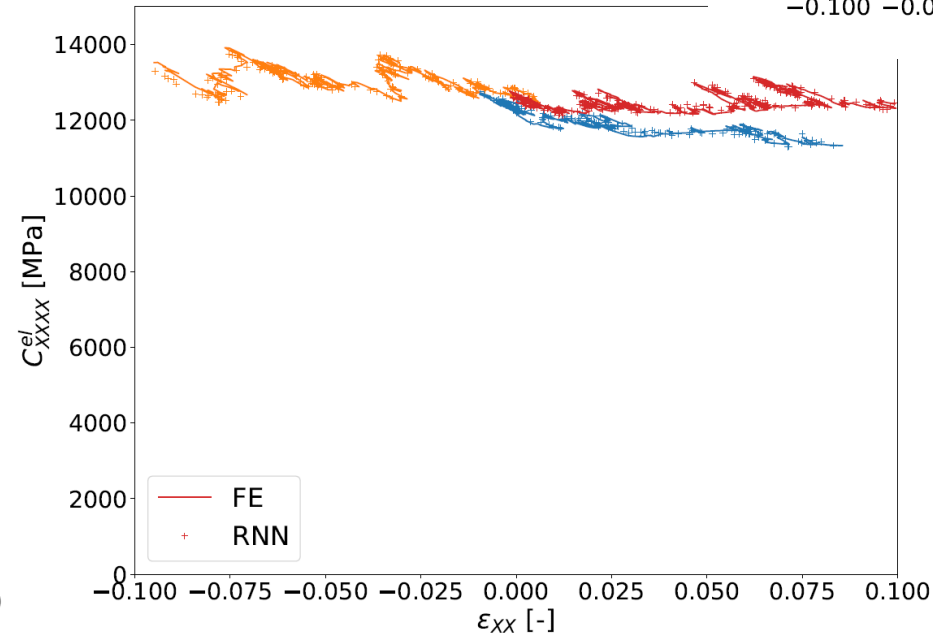
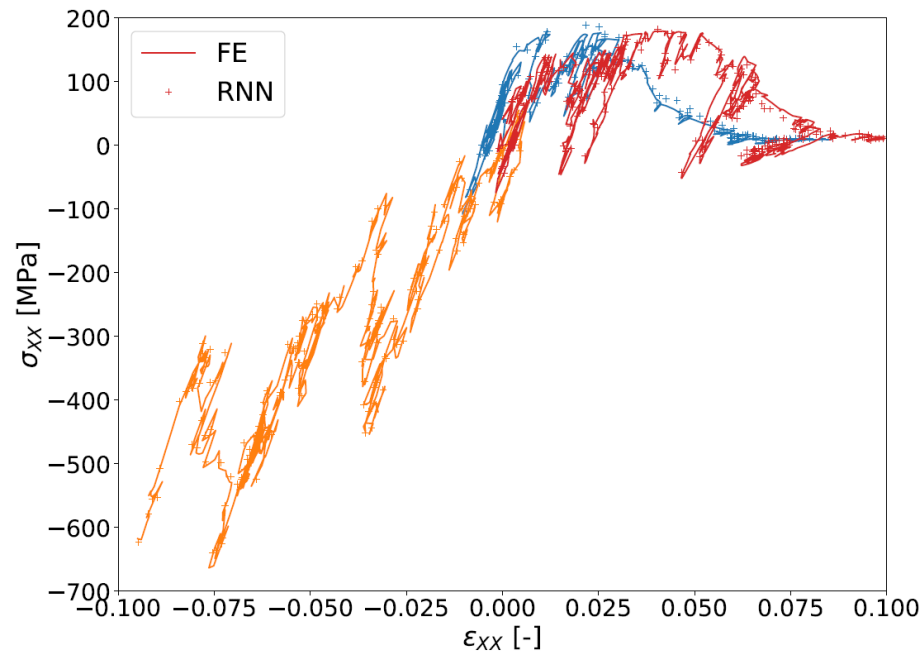


The training database

- I. Non-local framework
- II. **Surrogate (RNN)**
- III. Multi-scale simulations

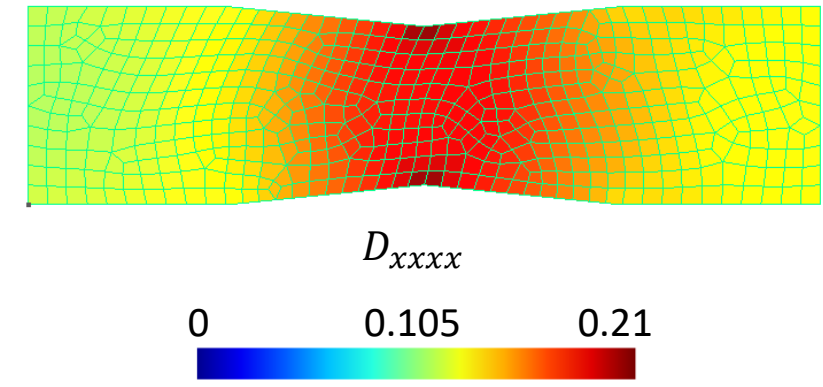
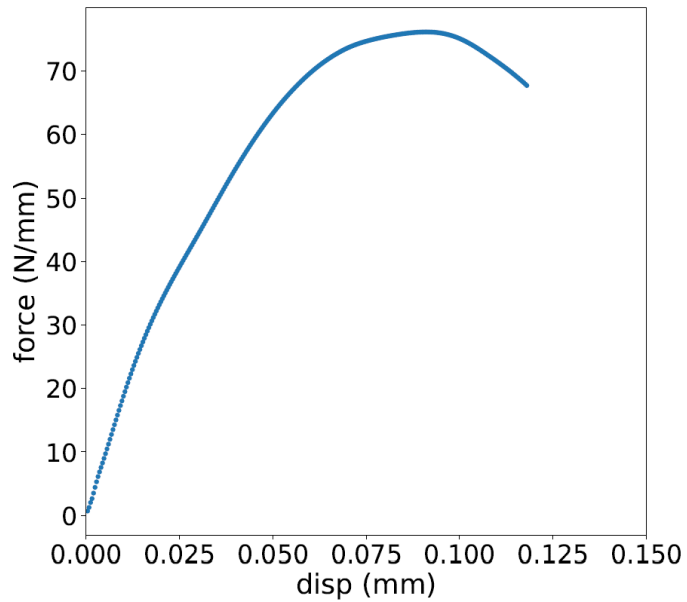
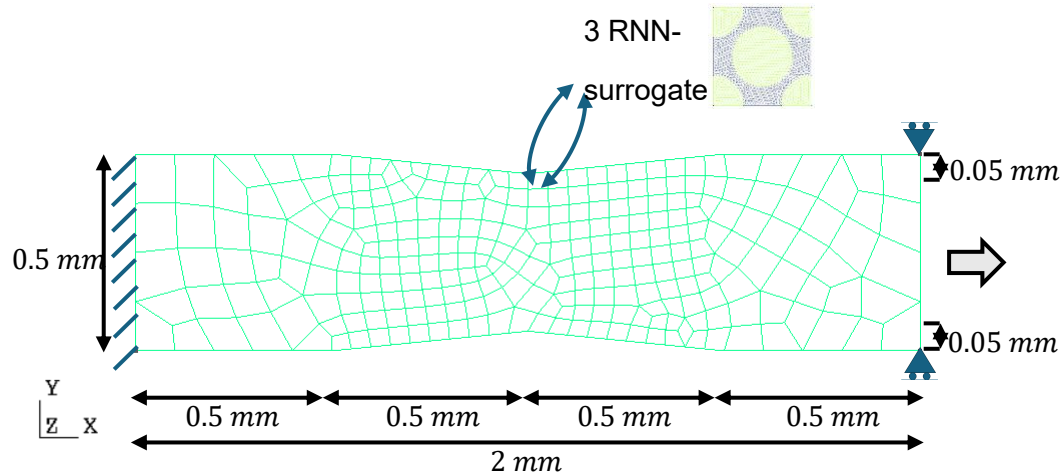


- 15 000 strain sequences generated
- 2/3 random paths, 1/3 cyclic paths
- FE simulations done, each taking $\sim 2\text{h}$

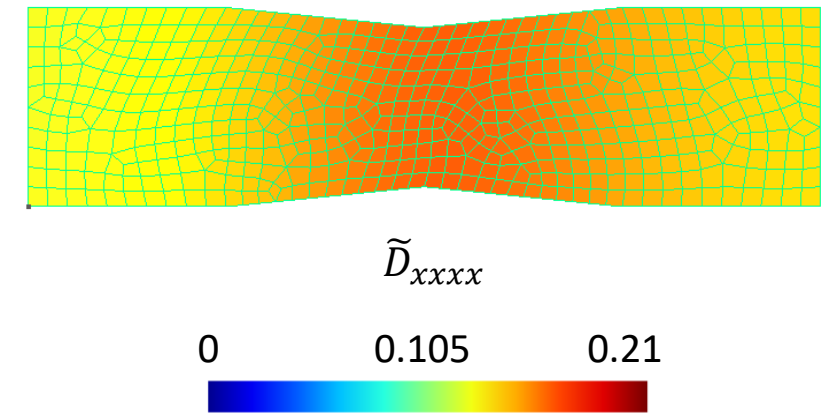


Multi-scale simulations

- I. Non-local framework
- II. Surrogate (RNN)
- III. Multi-scale simulations



(a) Local Damage



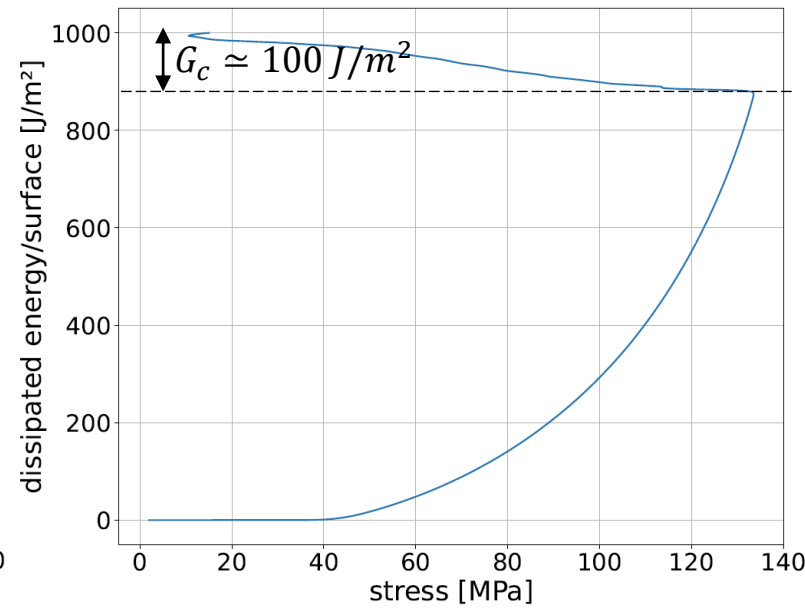
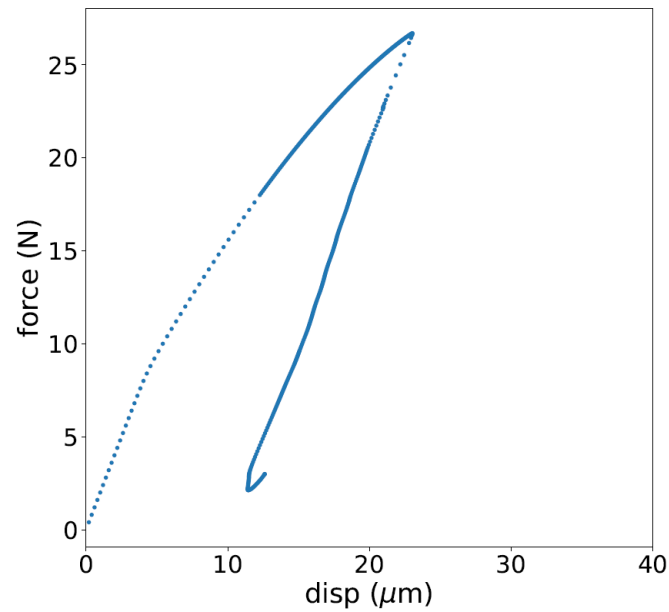
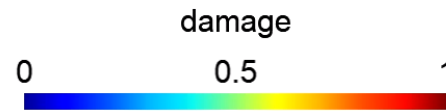
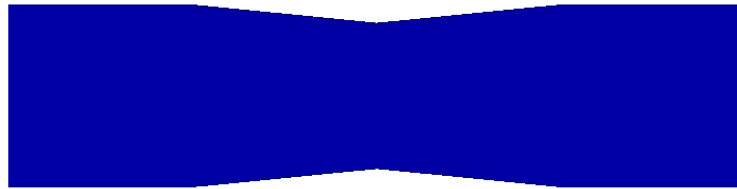
(b) Non-local Damage

Recover the composite behaviour

- I. Non-local framework
- II. Surrogate (RNN)
- III. Multi-scale simulations

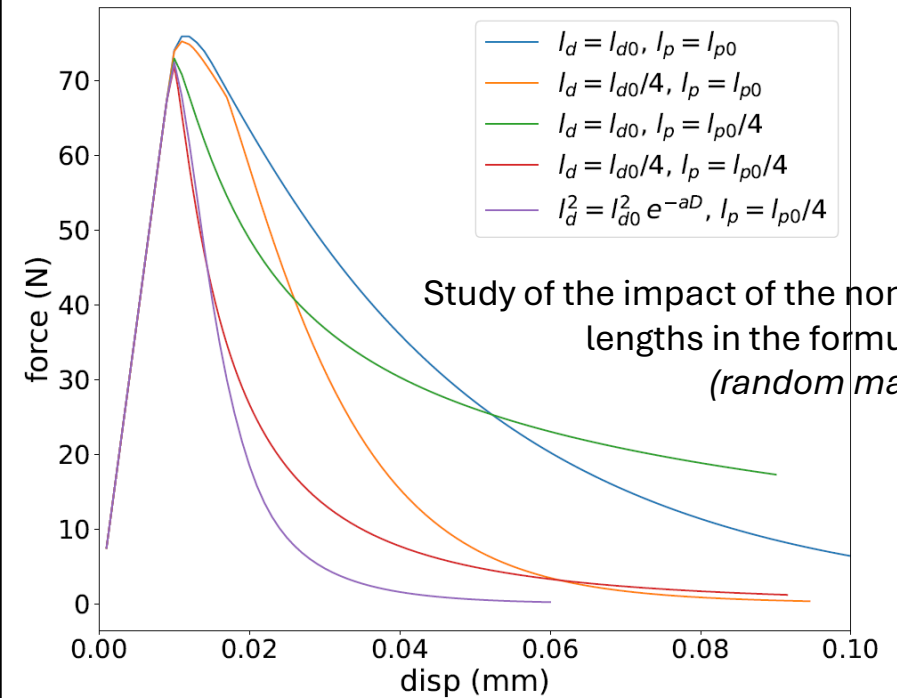
DNS simulation

length=800 μm



Goal: recover the results with the surrogate

→ by **tuning the non-local lengths** to have the same **force-displacement curve** as DNS



→ if same force-displacement curve, **automatically same G_c**

Next steps

- Recover the composite behaviour taken as an application
 - by tuning the non-local lengths
 - (the hope is not to have them too small to avoid thin meshes)
- Reduce the number of non-local variables
 - (to improve time-cost)
 - harmonic-analysis of the damage [1]

[1] 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