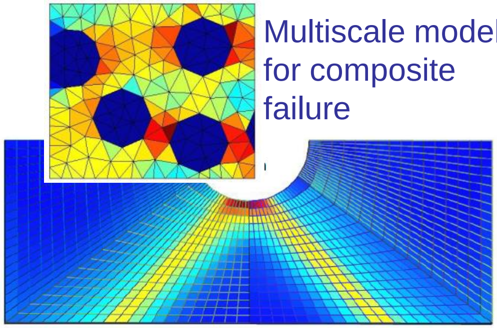
Multi-scale modelling

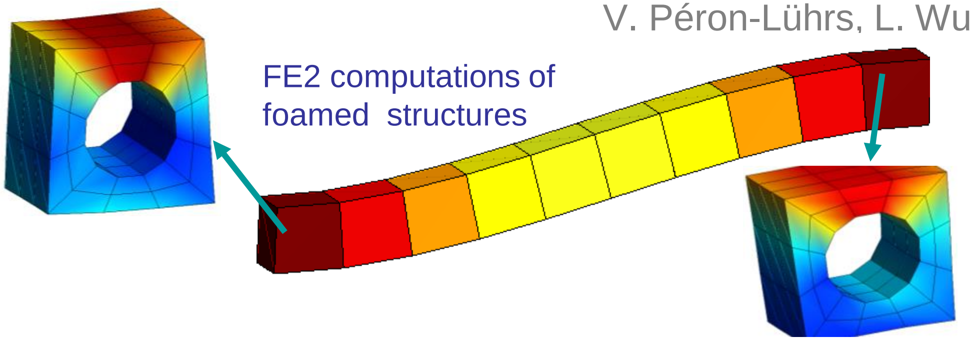
Ludovic Noels

G. Becker, S. Mulay, V.-D. Nguyen,

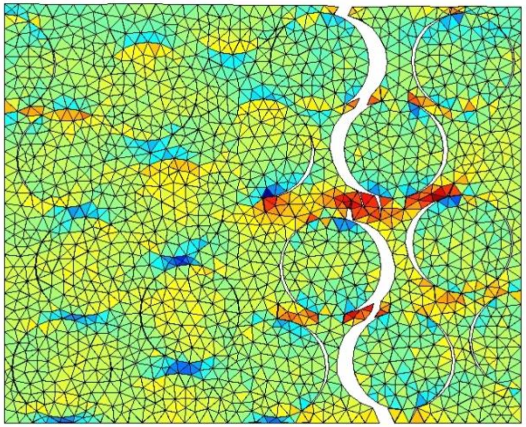
V. Péron-Lührs, L. Wu



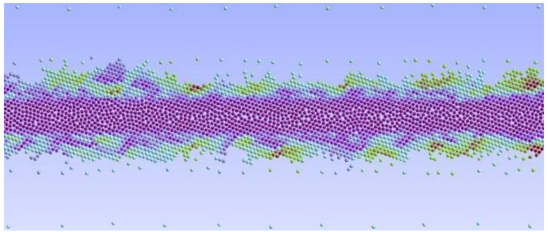
Multiscale models for composite failure



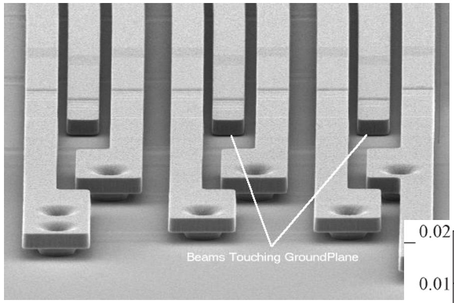
FE2 computations of foamed structures

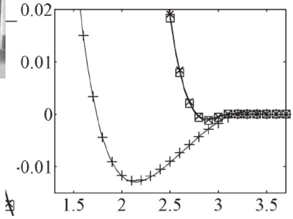


DG-based fracture framework



QC method for grain-boundary sliding





Stiction failure in a MEMS sensor (picture Sandia National Laboratories)

Content

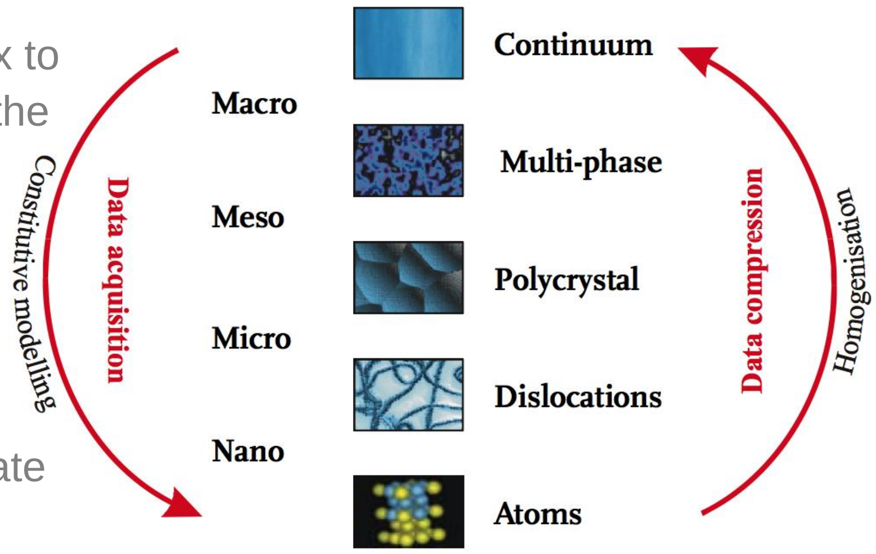
- Introduction
  - Multi-scale modelling: Why?
  - Multi-scale modelling: How?

- Mean-Field-Homogenization with non-local damage

- Conclusions

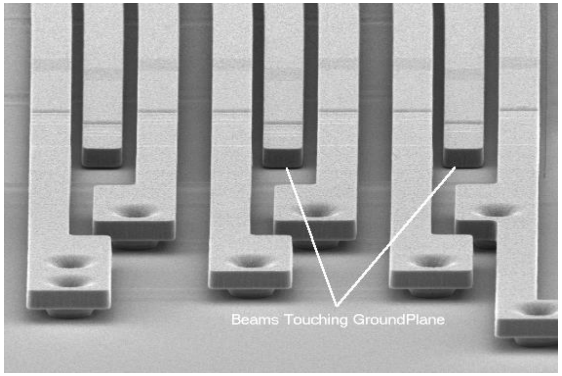
Multi-scale modelling: Why?

- Limitations of one-scale models
  - Physics at the micro-scale is too complex to be modelled by a simple material law at the macro-scale
    - Engineered materials
    - Multi-physics/scale problems
    - ….
    - See next slides
  - Lack of information of the micro-scale state during macro-scale deformations
    - Required to predict failure
    - …..
  - Effect of the micro-structure on the macro-structure response
    - Grain-size effect in metals
    - …
- Solution: multi-scale models



Multi-scale modelling: Why?

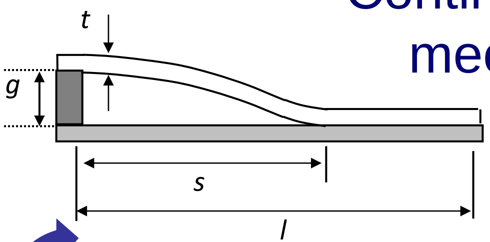
- Examples of multi-scale problems
  - Different physics at the different scales
  - Stiction (adhesion of MEMS)

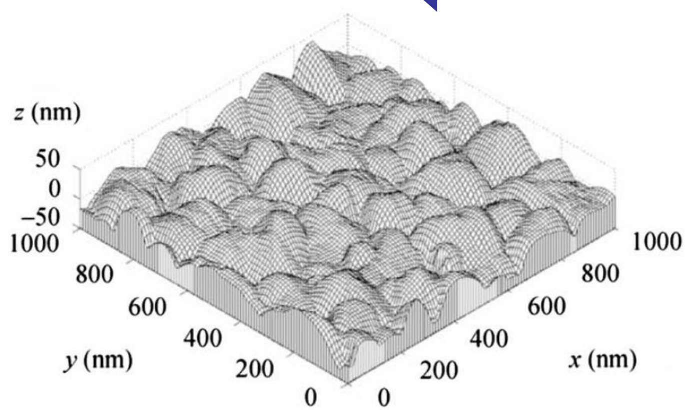


Stiction failure in a MEMS sensor

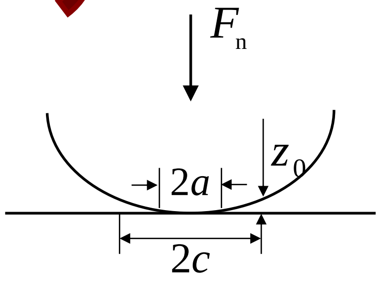
(Jeremy A.Walraven Sandia National Laboratories. Albuquerque, NM USA)

Continuum solid mechanics





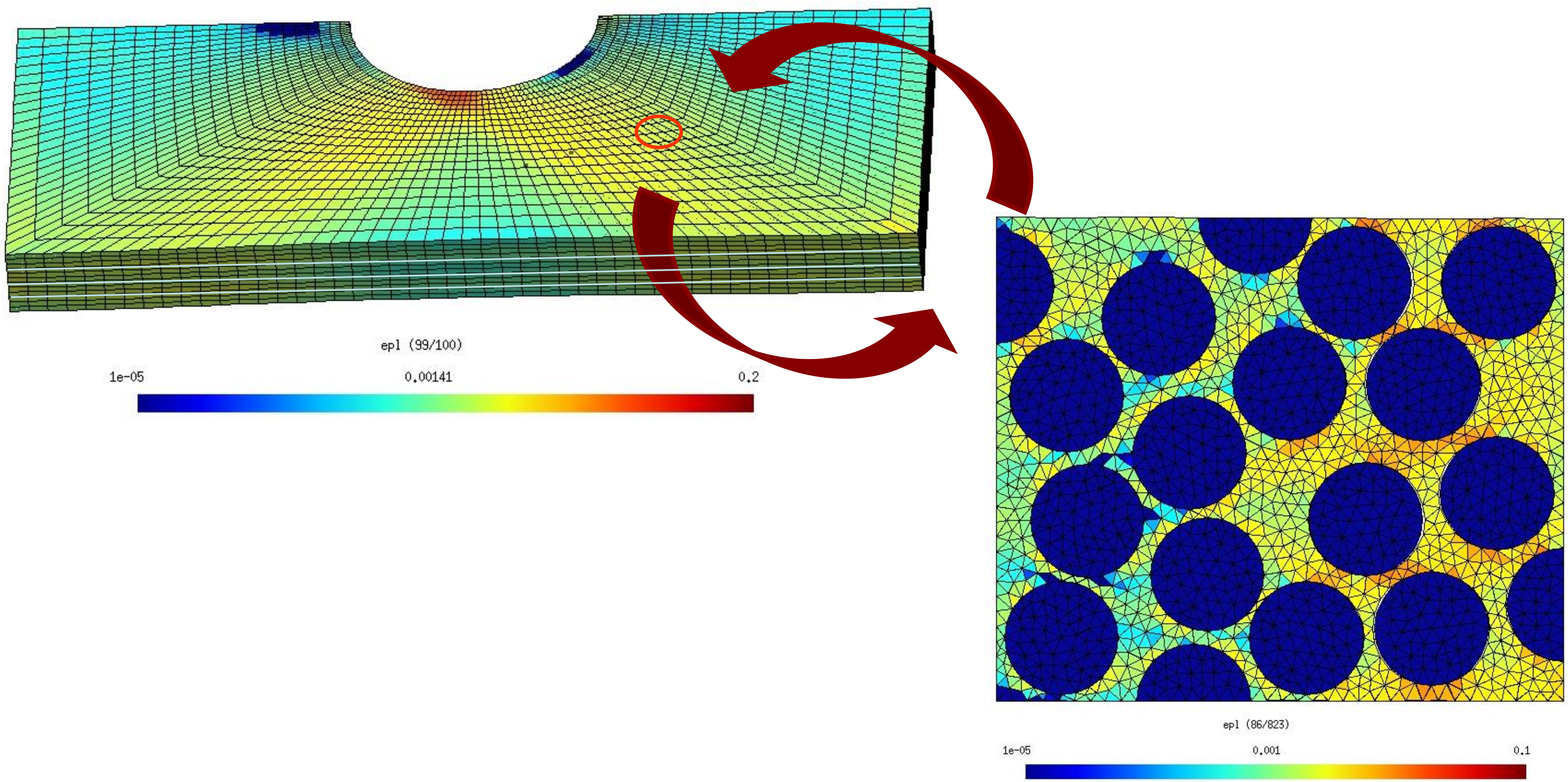
Statistical representation of rough surfaces



Van der Waals/capillary/Hertz forces at the asperity level

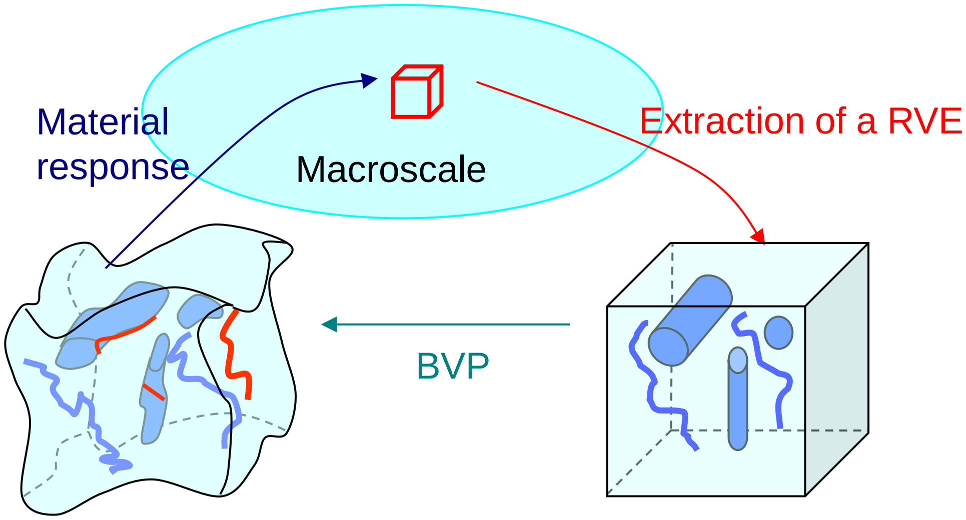
Multi-scale modelling: Why?

- Examples of multi-scale problems (2)
  - Continuum solid mechanics at the different scales
  - Non-linear response of $[-45_2/45_2]_S$ composites



Multi-scale modelling: How?

- Principle
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The micro-scale problem (Representative Volume Element)
  - Scale transitions coupling the two scales
    - Downscaling: transfer of macro-scale quantities (e.g. strain) to the micro-scale to determine the equilibrium state of the Boundary Value Problem
    - Upscaling: constitutive law (e.g. stress) for the macro-scale problem is determined from the micro-scale problem resolution

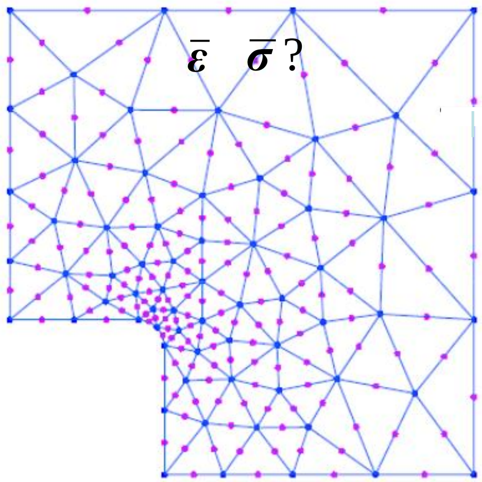


Assumptions:

$L_{macro} >> L_{RVE} >> L_{micro}$

Multi-scale modelling: How?

- Computational technique: FE^2
  - Macro-scale
    - FE model
    - At one integration point $\bar{\boldsymbol{\varepsilon}}$ is know, $\bar{\boldsymbol{\sigma}}$ is sought



Université de Liège

- Computational technique: FE^2
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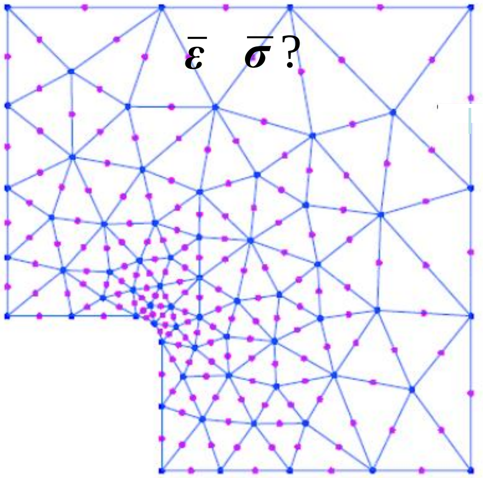
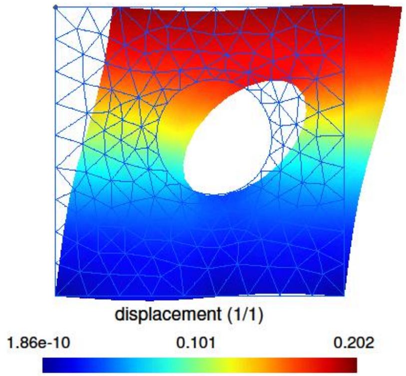
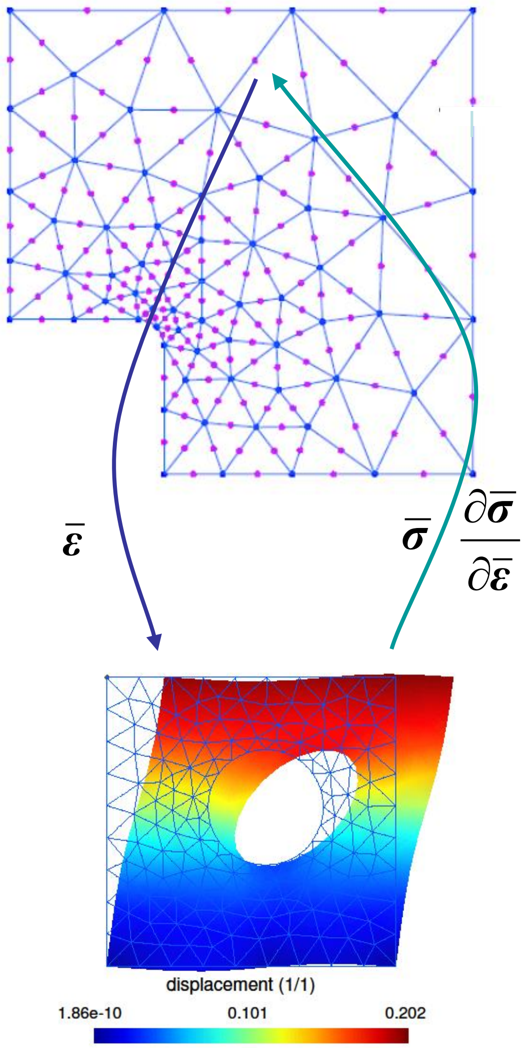


  - Micro-scale
    - Usual 3D finite elements
    - Periodic boundary conditions



Multi-scale modelling: How?

- Computational technique: FE^2
  - Macro-scale
    - FE model
    - At one integration point $\bar{\varepsilon}$ is know, $\bar{\sigma}$ is sought
  - Transition
    - Downscaling: $\bar{\varepsilon}$ is used to define the BCs
    - Upscaling: $\bar{\sigma}$ is known from the reaction forces
  - Micro-scale
    - Usual 3D finite elements
    - Periodic boundary conditions



Multi-scale modelling: How?

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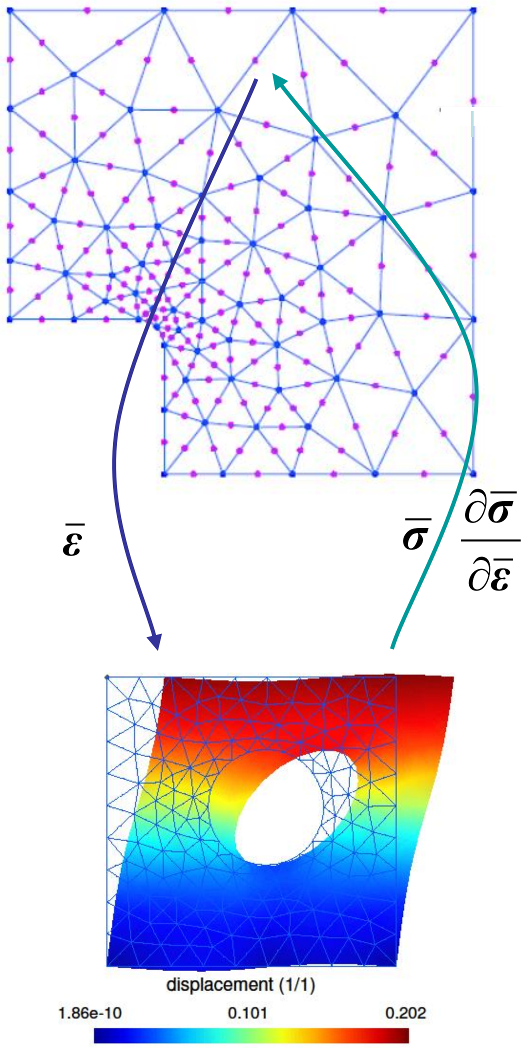
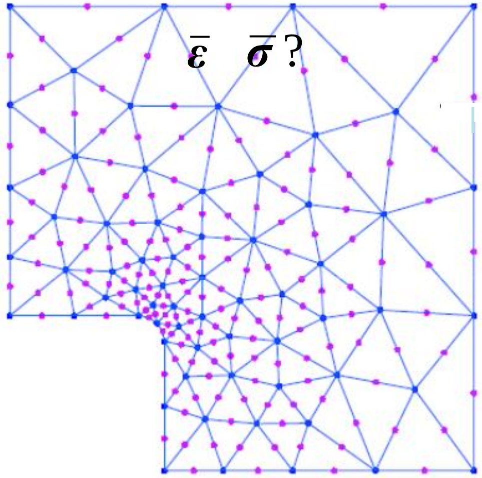
    - Upscaling: $\bar{\sigma}$ is known from the reaction forces
  - Micro-scale
    - Usual 3D finite elements
    - Periodic boundary conditions
  - Advantages
    - Accuracy
    - Generality
  - Drawback
    - Computational time



Ghosh S et al. 95, Kouznetsova et al. 2002, Geers et al. 2010, …

Multi-scale modelling: How?

- Mean-Field Homogenization
  - Macro-scale
    - FE model
    - At one integration point $\bar{\boldsymbol{\varepsilon}}$ is know, $\bar{\boldsymbol{\sigma}}$ is sought



Multi-scale modelling: How?

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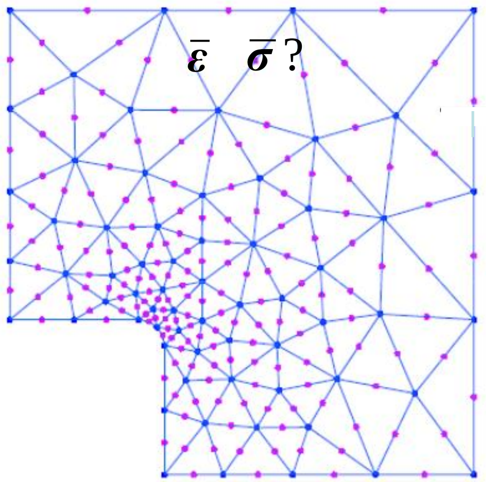
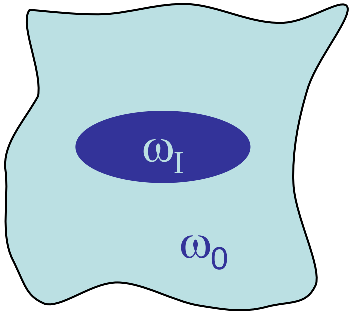
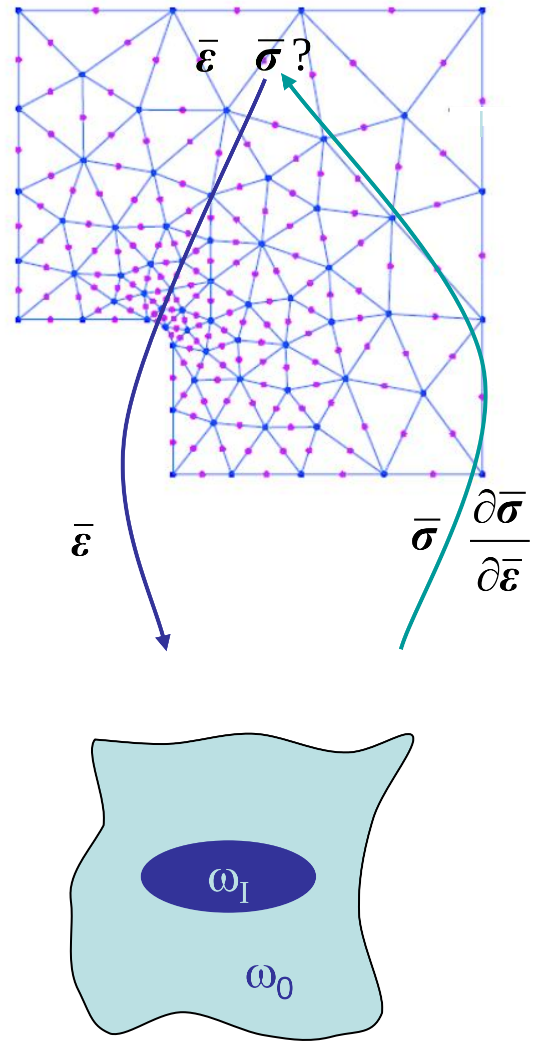


  - Micro-scale
    - Semi-analytical model
    - Predict composite meso-scale response
    - From components material models



Multi-scale modelling: How?

- Mean-Field Homogenization
  - Macro-scale
    - FE model
    - At one integration point $\bar{\boldsymbol{\varepsilon}}$ is know, $\bar{\boldsymbol{\sigma}}$ is sought
  - Transition
    - Downscaling: $\bar{\boldsymbol{\varepsilon}}$ is used as input of the MFH model
    - Upscaling: $\bar{\boldsymbol{\sigma}}$ is the output of the MFH model
  - Micro-scale
    - Semi-analytical model
    - Predict composite meso-scale response
    - From components material models



Multi-scale modelling: How?

- Mean-Field Homogenization
  - Macro-scale
    - FE model
    - At one integration point $\bar{\varepsilon}$ is know, $\bar{\sigma}$ is sought
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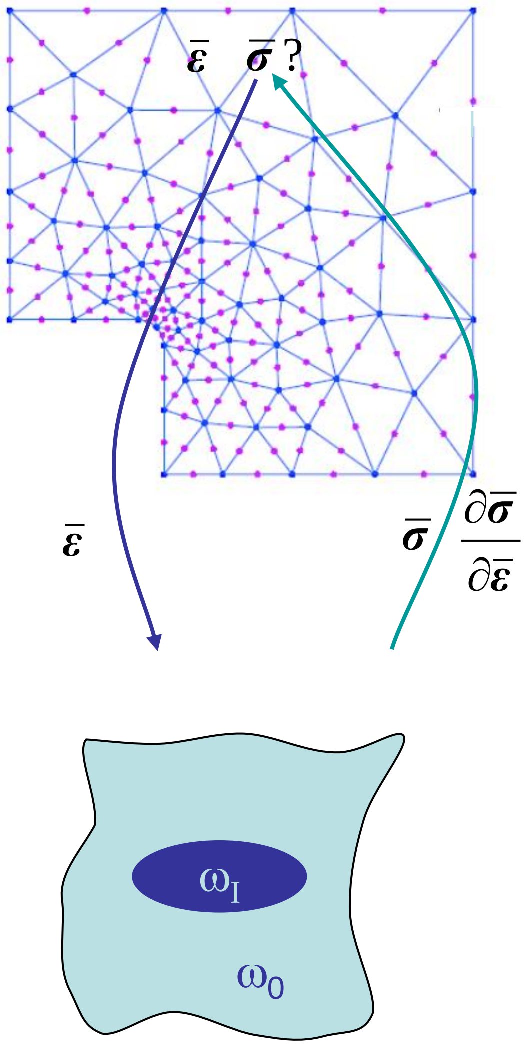
    - Downscaling: $\bar{\varepsilon}$ is used as input of the MFH model
    - Upscaling: $\bar{\sigma}$ is the output of the MFH model
  - Micro-scale
    - Semi-analytical model
    - Predict composite meso-scale response
    - From components material models
  - Advantages
    - Computationally efficient
    - Easy to integrate in a FE code (material model)
  - Drawbacks
    - Difficult to formulate in an accurate way
      - Geometry complexity
      - Material behaviours complexity



Mori and Tanaka 73, Hill 65, Ponte Castañeda 91, Suquet 95, Doghri et al 03, Lahellec et al. 11, Brassart et al. 12, …

- Semi analytical Mean-Field Homogenization
  - Based on the averaging of the fields

$$\langle a \rangle = \frac{1}{V}\int_V a(\boldsymbol{X})\,\mathrm{d}V$$

  - Meso-response
    - From the volume ratios ($v_0 + v_\mathrm{I} = 1$)

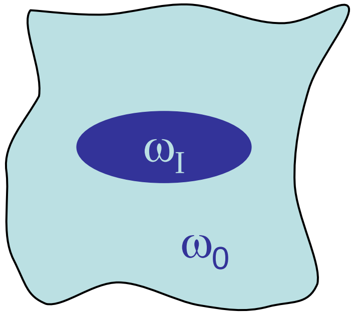
$$\begin{cases} \bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle = v_0 \langle \boldsymbol{\sigma} \rangle_{\omega_0} + v_\mathrm{I} \langle \boldsymbol{\sigma} \rangle_{\omega_\mathrm{I}} = v_0 \boldsymbol{\sigma}_0 + v_\mathrm{I} \boldsymbol{\sigma}_\mathrm{I} \\ \bar{\boldsymbol{\varepsilon}} = \langle \boldsymbol{\varepsilon} \rangle = v_0 \langle \boldsymbol{\varepsilon} \rangle_{\omega_0} + v_\mathrm{I} \langle \boldsymbol{\varepsilon} \rangle_{\omega_\mathrm{I}} = v_0 \boldsymbol{\varepsilon}_0 + v_\mathrm{I} \boldsymbol{\varepsilon}_\mathrm{I} \end{cases}$$

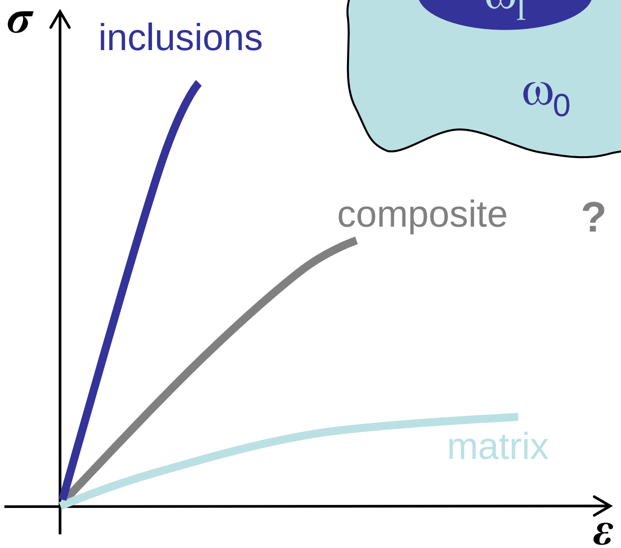
    - One more equation required

$$\boldsymbol{\varepsilon}_\mathrm{I} = \boldsymbol{B}^{\varepsilon} : \boldsymbol{\varepsilon}_0$$

  - Difficulty: find the adequate relations

$$\begin{cases} \boldsymbol{\sigma}_\mathrm{I} = f(\boldsymbol{\varepsilon}_\mathrm{I}) \\ \boldsymbol{\sigma}_0 = f(\boldsymbol{\varepsilon}_0) \\ \boldsymbol{\varepsilon}_\mathrm{I} = \boldsymbol{B}^{\varepsilon} : \boldsymbol{\varepsilon}_0 \end{cases} \qquad \boldsymbol{B}^{\varepsilon} \; ?$$





Multi-scale modelling: How?

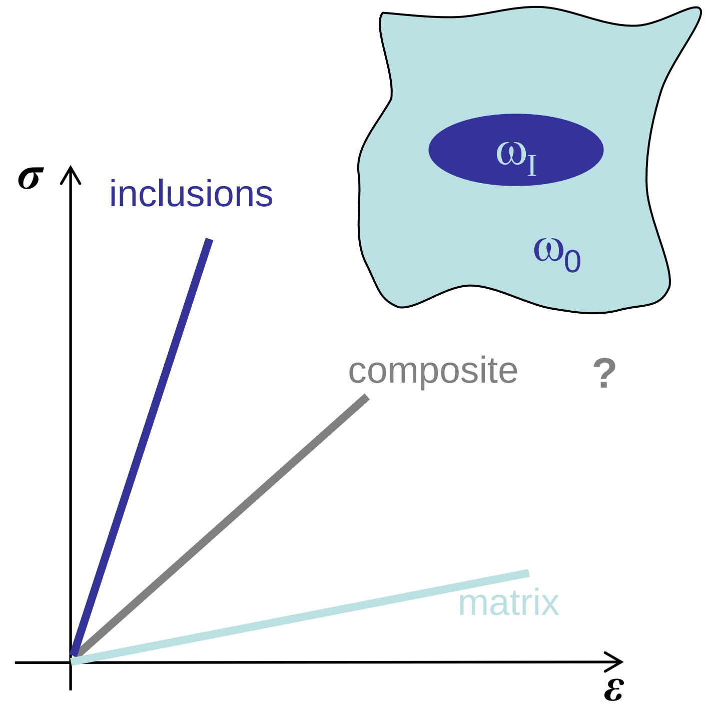
- Mean-Field Homogenization for linear materials
  - System of equations
    - From the volume ratios ($v_0 + v_{\mathrm{I}} = 1$)

$$\begin{cases} \bar{\boldsymbol{\sigma}} = v_0 \boldsymbol{\sigma}_0 + v_{\mathrm{I}} \boldsymbol{\sigma}_{\mathrm{I}} \\ \bar{\boldsymbol{\varepsilon}} = v_0 \boldsymbol{\varepsilon}_0 + v_{\mathrm{I}} \boldsymbol{\varepsilon}_{\mathrm{I}} \end{cases}$$

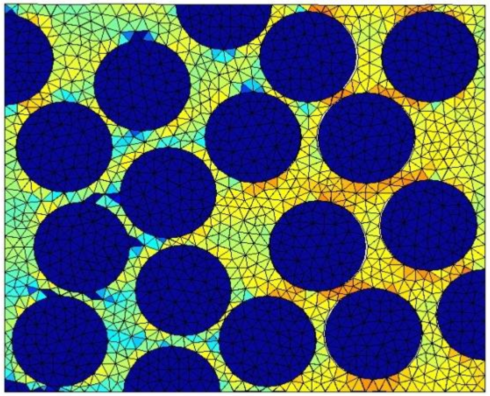
    - Assume linear behaviours

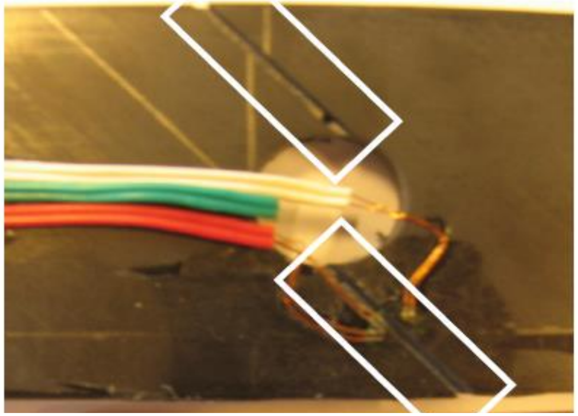
$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{I}} = \bar{\boldsymbol{C}}_{\mathrm{I}} : \boldsymbol{\varepsilon}_{\mathrm{I}} \\ \boldsymbol{\sigma}_0 = \bar{\boldsymbol{C}}_0 : \boldsymbol{\varepsilon}_0 \end{cases}$$

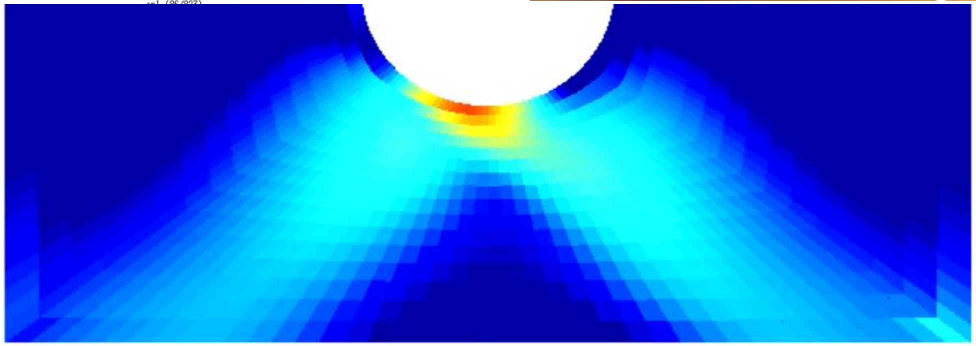
    - Relation between average strains $\boldsymbol{\varepsilon}_{\mathrm{I}} = \boldsymbol{B}^{\varepsilon} : \boldsymbol{\varepsilon}_0$



  - Single inclusion problem from Eshelby tensor $\boldsymbol{S}$
    - $\boldsymbol{\varepsilon}_{\mathrm{I}} = \boldsymbol{H}^{\varepsilon}(I, \bar{\boldsymbol{C}}_0, \bar{\boldsymbol{C}}_{\mathrm{I}}) : \varepsilon^{\infty}$ with $\boldsymbol{H}^{\varepsilon} = [\boldsymbol{I} + \boldsymbol{S} : \bar{\boldsymbol{C}}_0^{-1} : (\bar{\boldsymbol{C}}_1 - \bar{\boldsymbol{C}}_0)]^{-1}$
    - Results from a phase transformation analysis
  - Multiple inclusions problem
    - $\boldsymbol{\varepsilon}_{\mathrm{I}} = \boldsymbol{B}^{\varepsilon}\left(\mathrm{I}, \bar{\boldsymbol{C}}_0, \bar{\boldsymbol{C}}_{\mathrm{I}}\right) : \boldsymbol{\varepsilon}_0$
    - Mori-Tanaka assumption $\boldsymbol{\varepsilon}^{\infty} = \boldsymbol{\varepsilon}_0 \Rightarrow \boldsymbol{B}^{\varepsilon} = \boldsymbol{H}^{\varepsilon}$







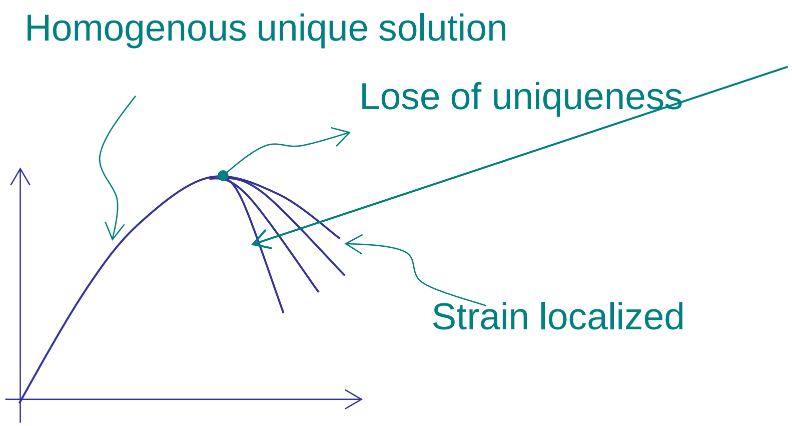
Non-local damage-enhanced mean-field-homogenization

L. Wu (ULg), L. Noels (ULg), L. Adam (e-Xstream), I. Doghri (UCL)

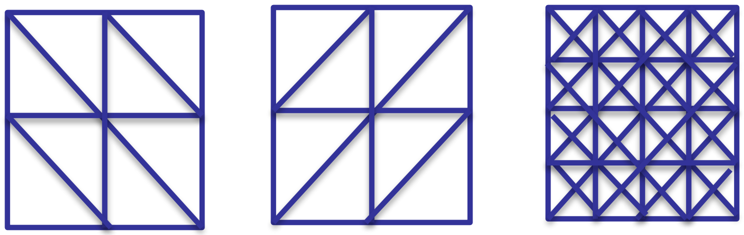
SIMUCOMP The research has been funded by the Walloon Region under the agreement no 1017232 (CT-EUC 2010-10-12) in the context of the ERA-NET +, Matera + framework.

Non-local damage mean-field-homogenization

- Finite element solutions for strain softening problems suffer from:
  - The loss the uniqueness and strain localization
  - Mesh dependence



The numerical results change with the size of mesh and direction of mesh



The numerical results change without convergence

- Implicit non-local approach [Peerlings et al 96, Geers et al 97, …]
  - A state variable is replaced by a non-local value reflecting the interaction between neighboring material points

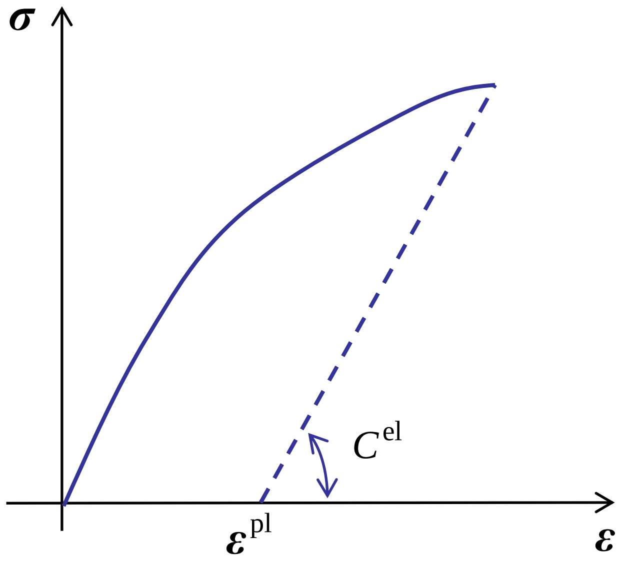
$$\tilde{a}(\boldsymbol{x}) = \frac{1}{V_C}\int_{V_C} a(\boldsymbol{y}) w(\boldsymbol{y};\boldsymbol{x}) \mathrm{d}V$$

  - Use Green functions as weight $w(y; x)$

$$\Rightarrow \quad \tilde{a} - c\nabla^2\tilde{a} = a \quad \Rightarrow$$ New degrees of freedom

Non-local damage mean-field-homogenization

- Material models
  - Elasto-plastic material
    - Stress tensor $\boldsymbol{\sigma} = \boldsymbol{C}^{\text{el}} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{pl}})$
    - Yield surface $f(\boldsymbol{\sigma}, p) = \boldsymbol{\sigma}^{\text{eq}} - \sigma^{Y} - R(p) \leq 0$
    - Plastic flow $\Delta\boldsymbol{\varepsilon}^{\text{pl}} = \Delta p \boldsymbol{N}$ & $\boldsymbol{N} = \frac{\partial f}{\partial \boldsymbol{\sigma}}$
    - Linearization $\delta\boldsymbol{\sigma} = \boldsymbol{C}^{\text{alg}} : \delta\boldsymbol{\varepsilon}$



- Material models
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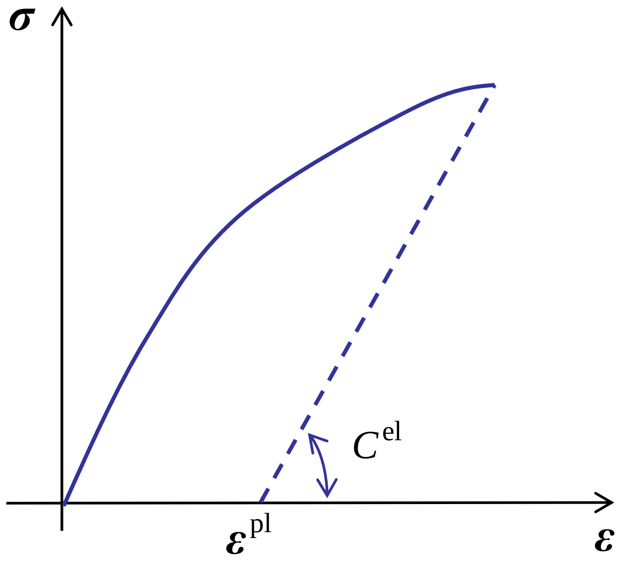
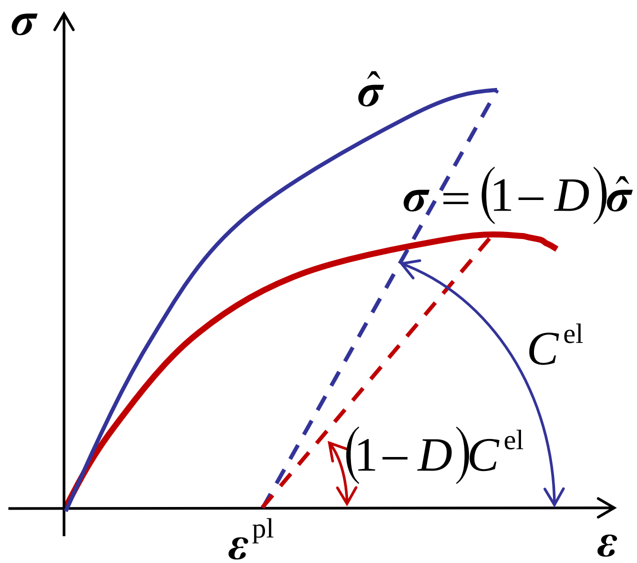
    - Linearization $\delta\boldsymbol{\sigma} = \boldsymbol{C}^{\text{alg}} : \delta\boldsymbol{\varepsilon}$
  - Local damage model
    - Apparent-effective stress tensors $\boldsymbol{\sigma} = (1 - D)\hat{\boldsymbol{\sigma}}$
    - Plastic flow in the effective stress space
    - Damage evolution $\Delta D = F_D(\boldsymbol{\varepsilon}, \Delta p)$





Non-local damage mean-field-homogenization

- Material models
  - Elasto-plastic material
    - Stress tensor $\boldsymbol{\sigma} = \boldsymbol{C}^{\mathrm{el}} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{pl}})$
    - Yield surface $f(\boldsymbol{\sigma}, p) = \boldsymbol{\sigma}^{\mathrm{eq}} - \sigma^{Y} - R(p) \leq 0$
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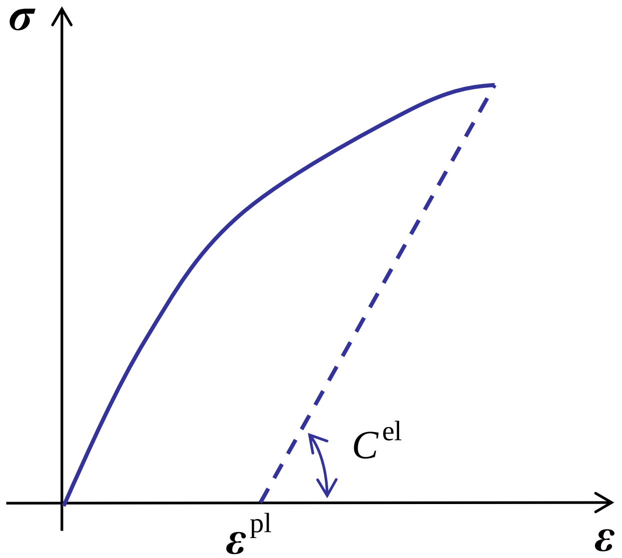
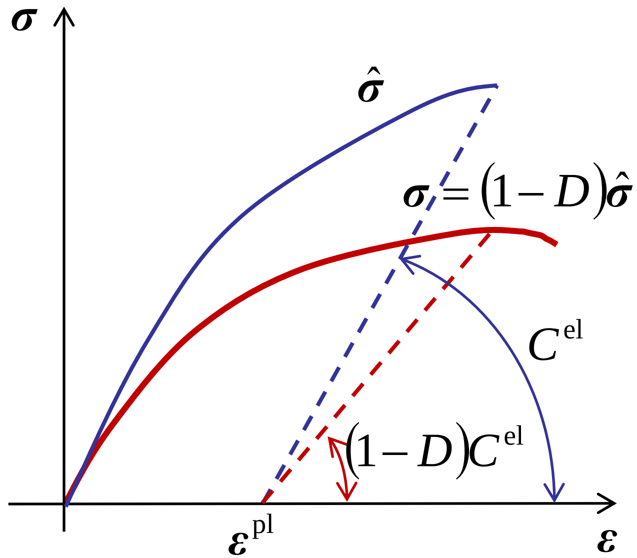
    - Apparent-effective stress tensors $\boldsymbol{\sigma} = (1 - D)\hat{\boldsymbol{\sigma}}$
    - Plastic flow in the effective stress space
    - Damage evolution $\Delta D = F_D(\boldsymbol{\varepsilon}, \Delta p)$
  - Non-Local damage model
    - Damage evolution $\Delta D = F_D(\boldsymbol{\varepsilon}, \Delta \tilde{p})$
    - Anisotropic governing equation $\tilde{p} - \nabla \cdot (\boldsymbol{c}_{\mathrm{g}} \cdot \nabla \tilde{p}) = p$
    - Linearization

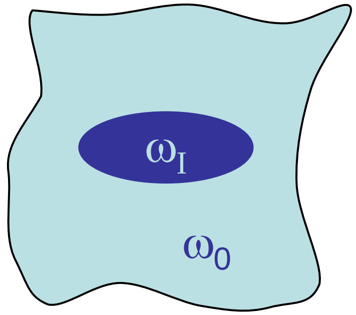
$$\delta\boldsymbol{\sigma} = \left[(1 - D)\boldsymbol{C}^{\mathrm{alg}} - \hat{\boldsymbol{\sigma}} \otimes \frac{\partial F_D}{\partial \boldsymbol{\varepsilon}} \right] : \delta\boldsymbol{\varepsilon} - \hat{\boldsymbol{\sigma}} \frac{\partial F_D}{\partial \tilde{p}} \delta\tilde{p}$$

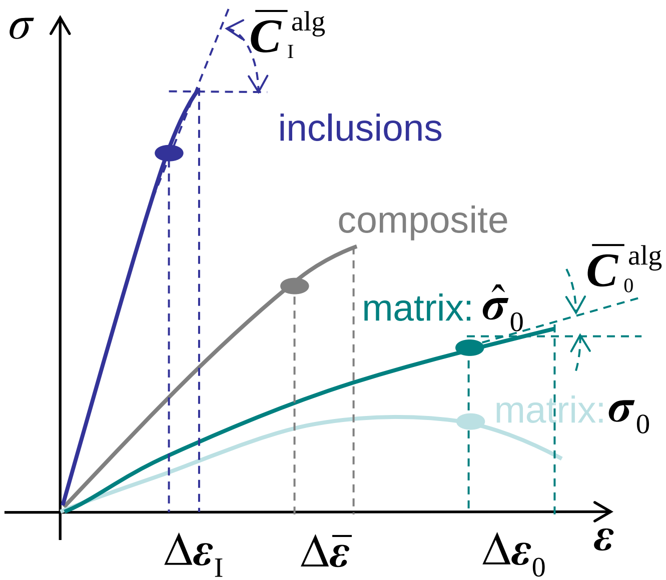




- Incremental-tangent model with damage in the matrix
  - From the volume ratios ($v_0 + v_I = 1$)

$$\begin{cases} \bar{\boldsymbol{\sigma}} = v_0 \boldsymbol{\sigma}_0 + v_I \boldsymbol{\sigma}_I \\ \bar{\boldsymbol{\varepsilon}} = v_0 \boldsymbol{\varepsilon}_0 + v_1 \boldsymbol{\varepsilon}_I \end{cases}$$





  - Non-linear phases behaviours
    - Elasto-plastic inclusions

$$\delta \boldsymbol{\sigma}_I = \bar{\boldsymbol{C}}_I^{\text{alg}} : \delta \boldsymbol{\varepsilon}_I$$

    - Non-local damaged matrix

$$\delta \boldsymbol{\sigma}_0 = \left[(1-D) \bar{\boldsymbol{C}}^{\text{alg}} - \hat{\boldsymbol{\sigma}}_0 \otimes \frac{\partial \bar{F}_D}{\partial \boldsymbol{\varepsilon}_0} \right] : \delta \boldsymbol{\varepsilon}_0 - \hat{\boldsymbol{\sigma}}_0 \frac{\partial \bar{F}_D}{\partial \tilde{p}} \delta \tilde{p}$$

    - Composite

$$\delta \bar{\boldsymbol{\sigma}} = v_I \bar{\boldsymbol{C}}_I^{\text{alg}} : \delta \boldsymbol{\varepsilon}_I + v_0 (1-D) \bar{\boldsymbol{C}}_0^{\text{alg}} : \delta \boldsymbol{\varepsilon}_0 - v_0 \hat{\boldsymbol{\sigma}}_0 \otimes \frac{\partial \bar{F}_D}{\partial \boldsymbol{\varepsilon}_0} : \delta \boldsymbol{\varepsilon}_0 - v_0 \hat{\boldsymbol{\sigma}}_0 \frac{\partial \bar{F}_D}{\partial \tilde{p}} \delta \tilde{p}$$

Mori-Tanaka on one loading interval: $\Delta \boldsymbol{\varepsilon}_I = \boldsymbol{B}^{\varepsilon} \left(\text{I}, (1-D) \bar{\boldsymbol{C}}_0^{\text{alg}}, \bar{\boldsymbol{C}}_I^{\text{alg}} \right) : \Delta \boldsymbol{\varepsilon}_0$

- Finite-element implementation
  - Strong form

$$\begin{cases} \nabla \cdot \bar{\boldsymbol{\sigma}}^T + \boldsymbol{f} = \boldsymbol{0} & \text{for the homogenized composite material} \\ \tilde{p} - \nabla \cdot \left(\boldsymbol{c}_\mathrm{g} \cdot \nabla \tilde{p} \right) = p & \text{for the matrix phase} \end{cases}$$

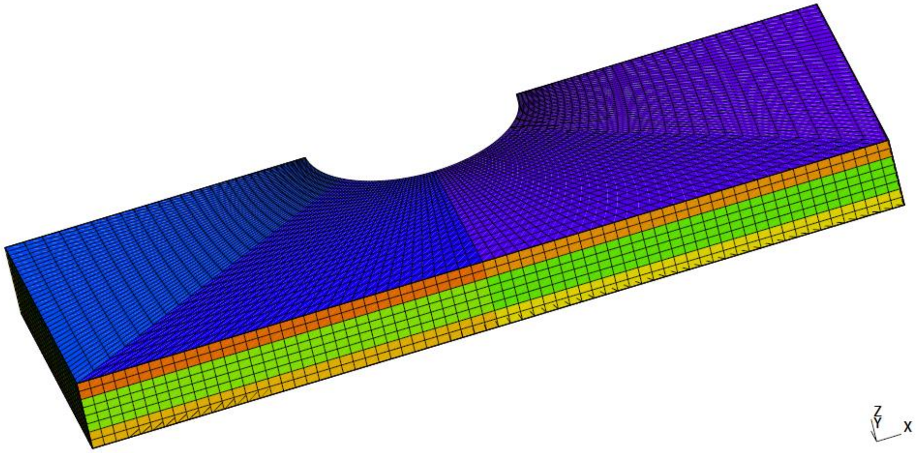
  - Boundary conditions

$$\begin{cases} \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{T} \\ \boldsymbol{n} \cdot \left(\boldsymbol{c}_\mathrm{g} \cdot \nabla \tilde{p} \right) = 0 \end{cases}$$

  - Finite-element discretization

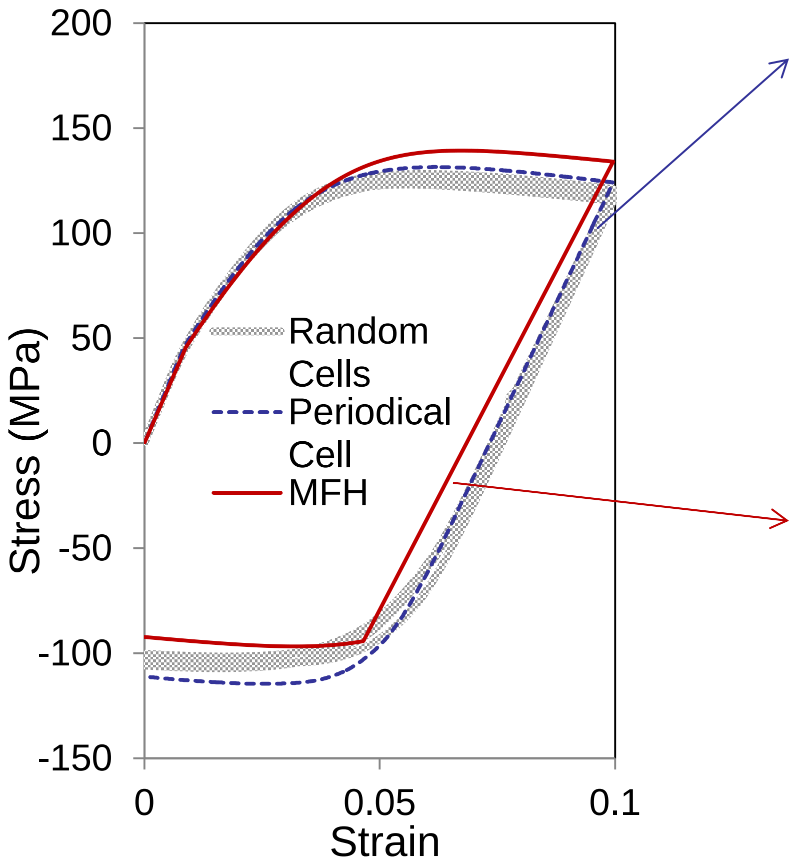
$$\begin{cases} \tilde{p} = N^a_{\tilde{p}} \tilde{\boldsymbol{p}}^a \\ \boldsymbol{u} = N^a_u \boldsymbol{u}^a \end{cases}$$

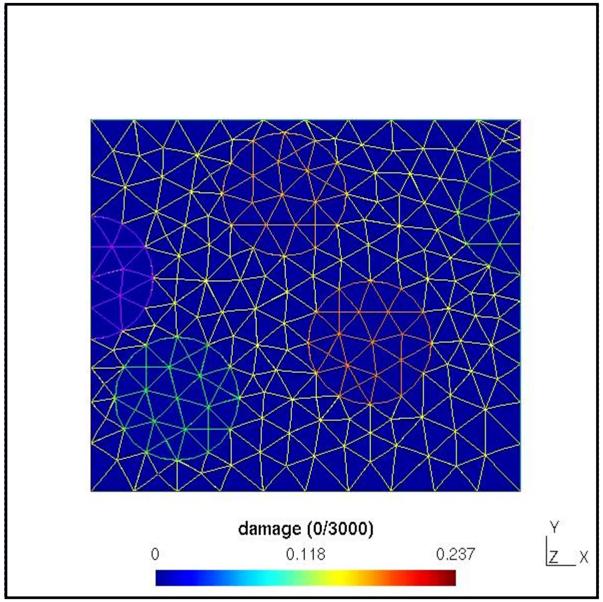
$$\Rightarrow \begin{bmatrix} \boldsymbol{K}_{uu} & \boldsymbol{K}_{u\tilde{p}} \\ \boldsymbol{K}_{\tilde{p}u} & \boldsymbol{K}_{u\tilde{p}} \end{bmatrix} \begin{bmatrix} d\boldsymbol{u} \\ d\tilde{\boldsymbol{p}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_\mathrm{ext} - \boldsymbol{F}_\mathrm{int} \\ \boldsymbol{F}_p - \boldsymbol{F}_{\tilde{p}} \end{bmatrix}$$

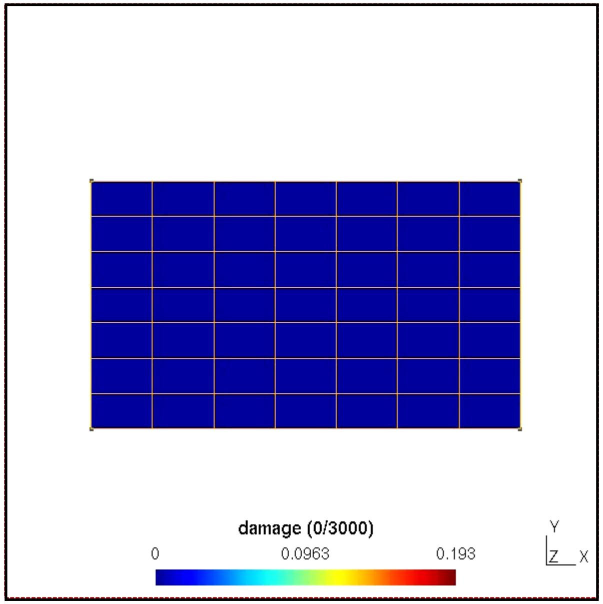


Non-local damage mean-field-homogenization

- DNS vs. FE/MFH
  - Fictitious composite
    - 30%-UD fibres
    - Elasto-plastic matrix with damage

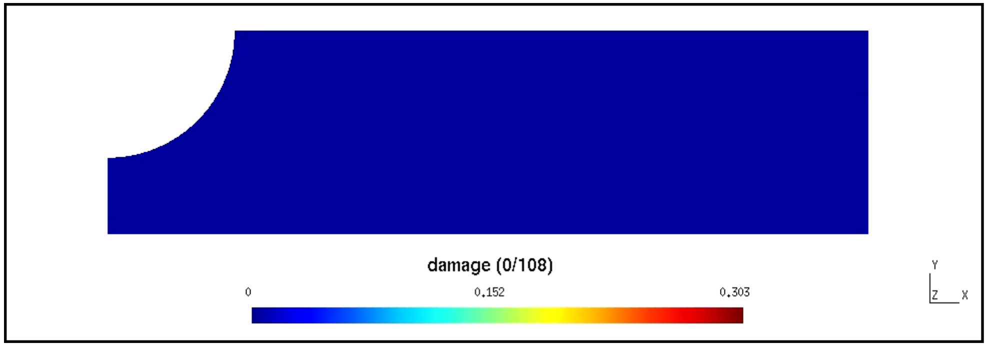


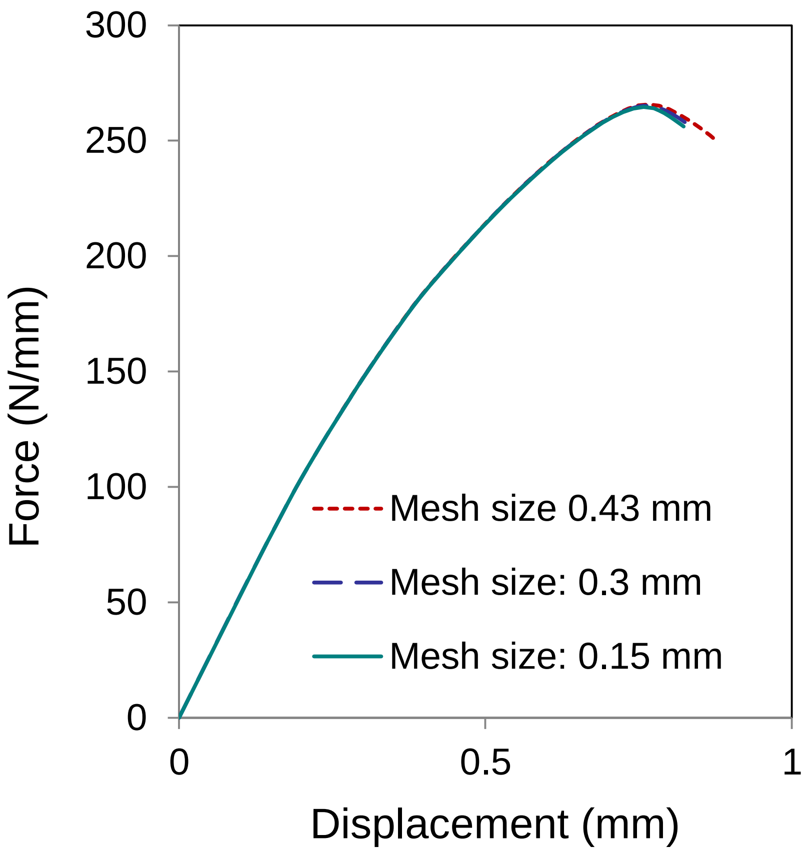




Non-local damage mean-field-homogenization

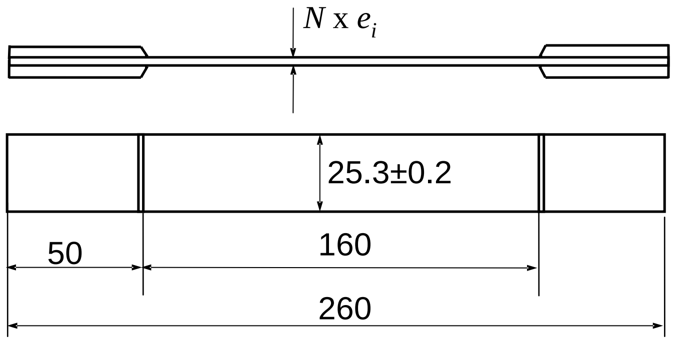
- Mesh-size effect
  - Fictitious composite
    - 30%-UD fibres
    - Elasto-plastic matrix with damage
  - Notched ply

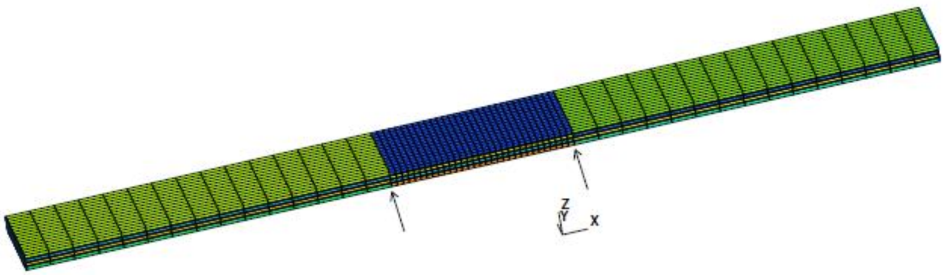


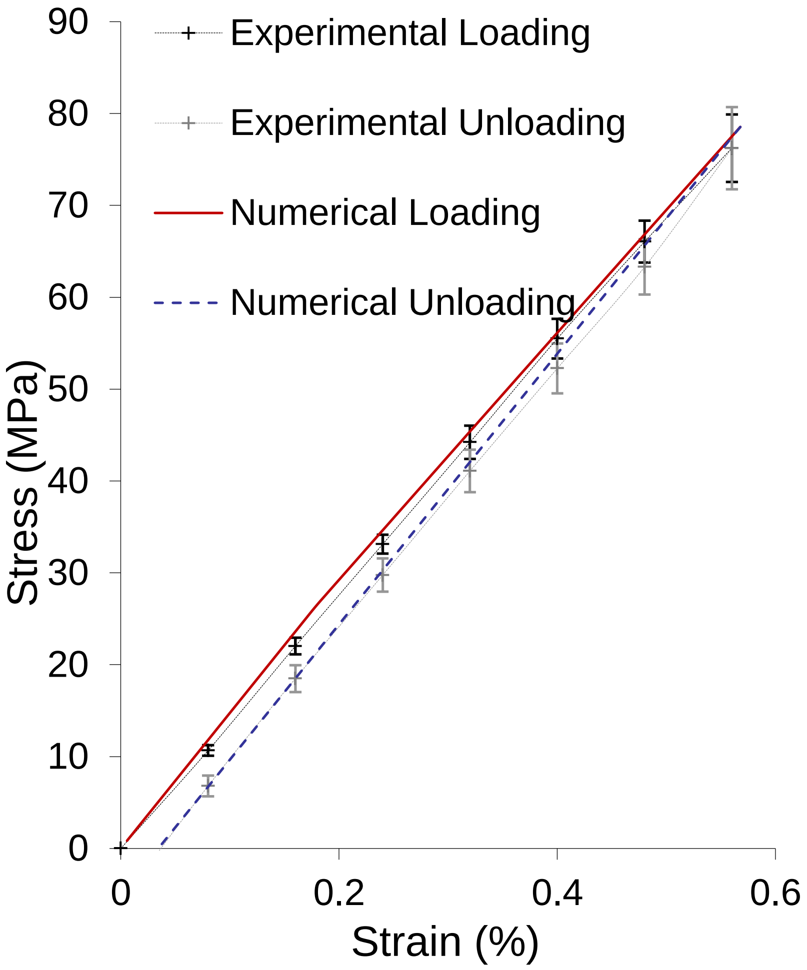


Non-local damage mean-field-homogenization

- Laminate: calibration
  - Carbon-fibres reinforced epoxy
    - 60%-UD fibres
    - Elasto-plastic matrix with damage
  - $[-45_2/45_2]_S$ staking sequence







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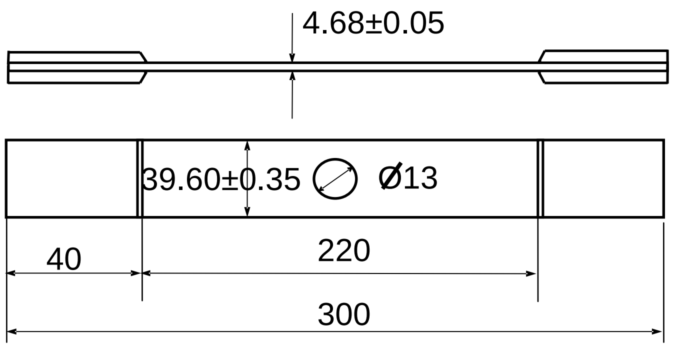
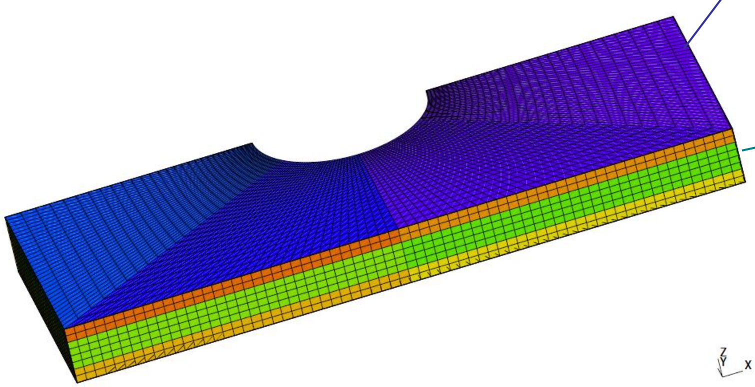
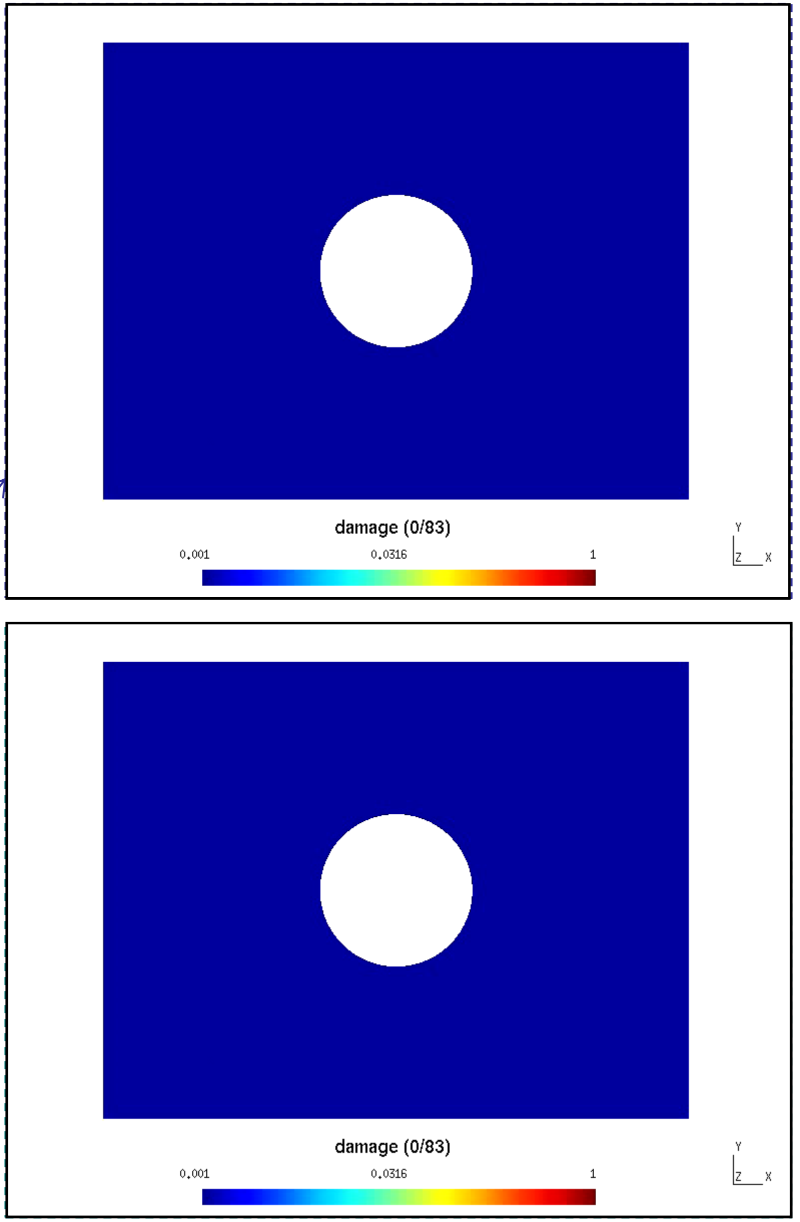
Non-local damage mean-field-homogenization

- Laminate plate with hole
  - Carbon-fibres reinforced epoxy
    - 60%-UD fibres
    - Elasto-plastic matrix with damage
  - $[-45_2/45_2]_S$ staking sequence

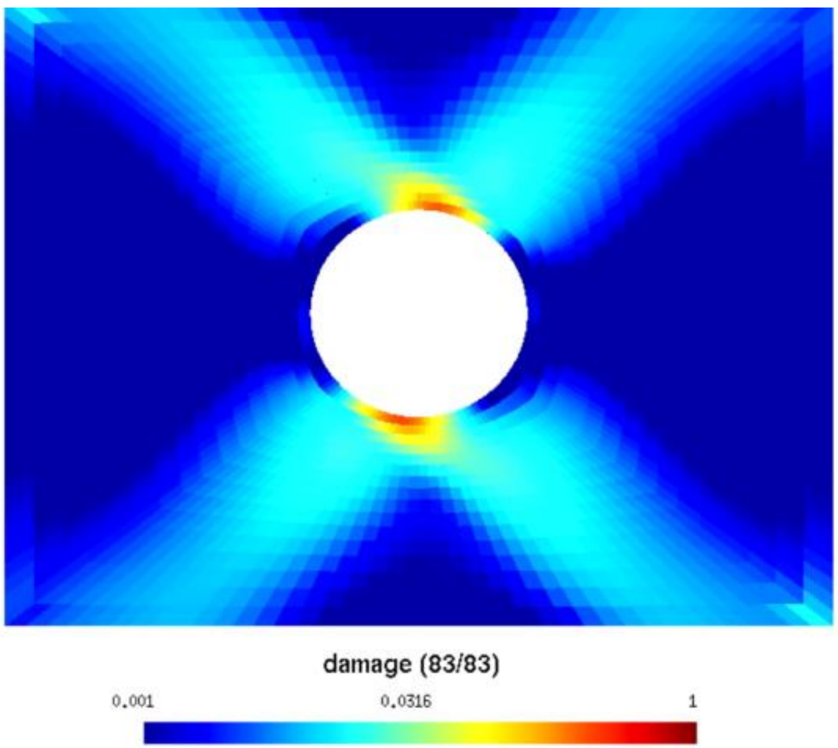


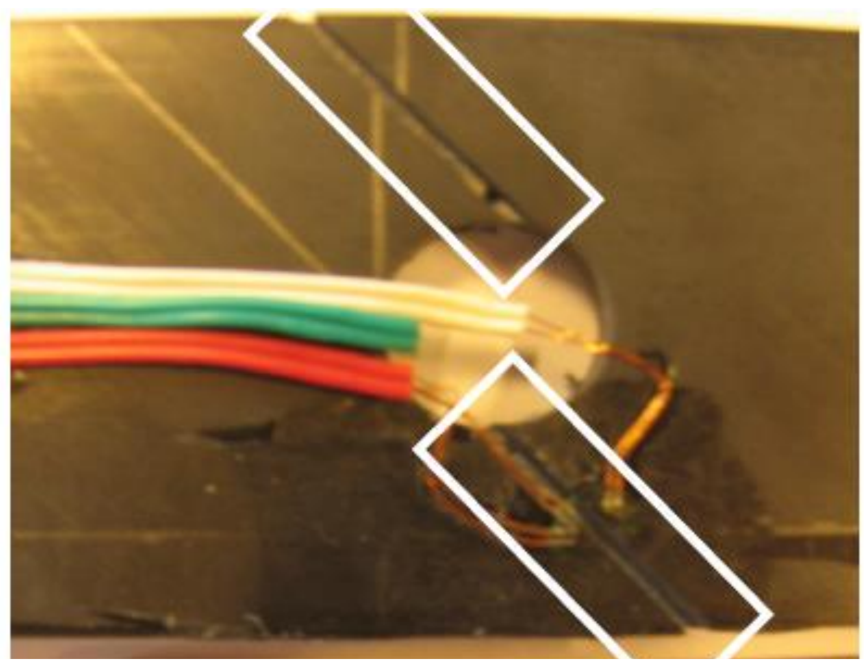




Non-local damage mean-field-homogenization

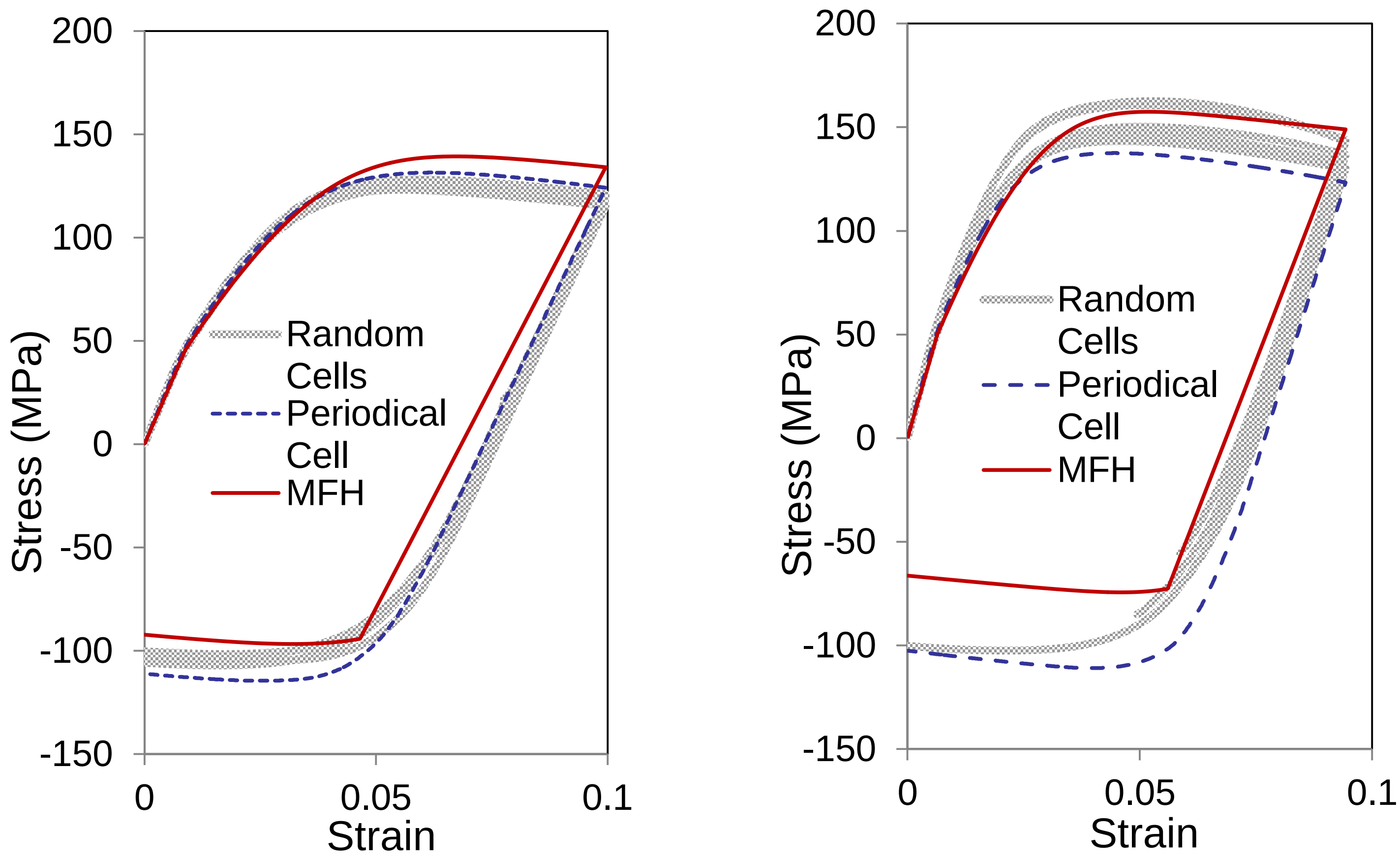
- Laminate plate with hole (2)
  - Carbon-fibres reinforced epoxy
    - 60%-UD fibres
    - Elasto-plastic matrix with damage
  - $[-45_2/45_2]_S$ staking sequence





Non-local damage mean-field-homogenization

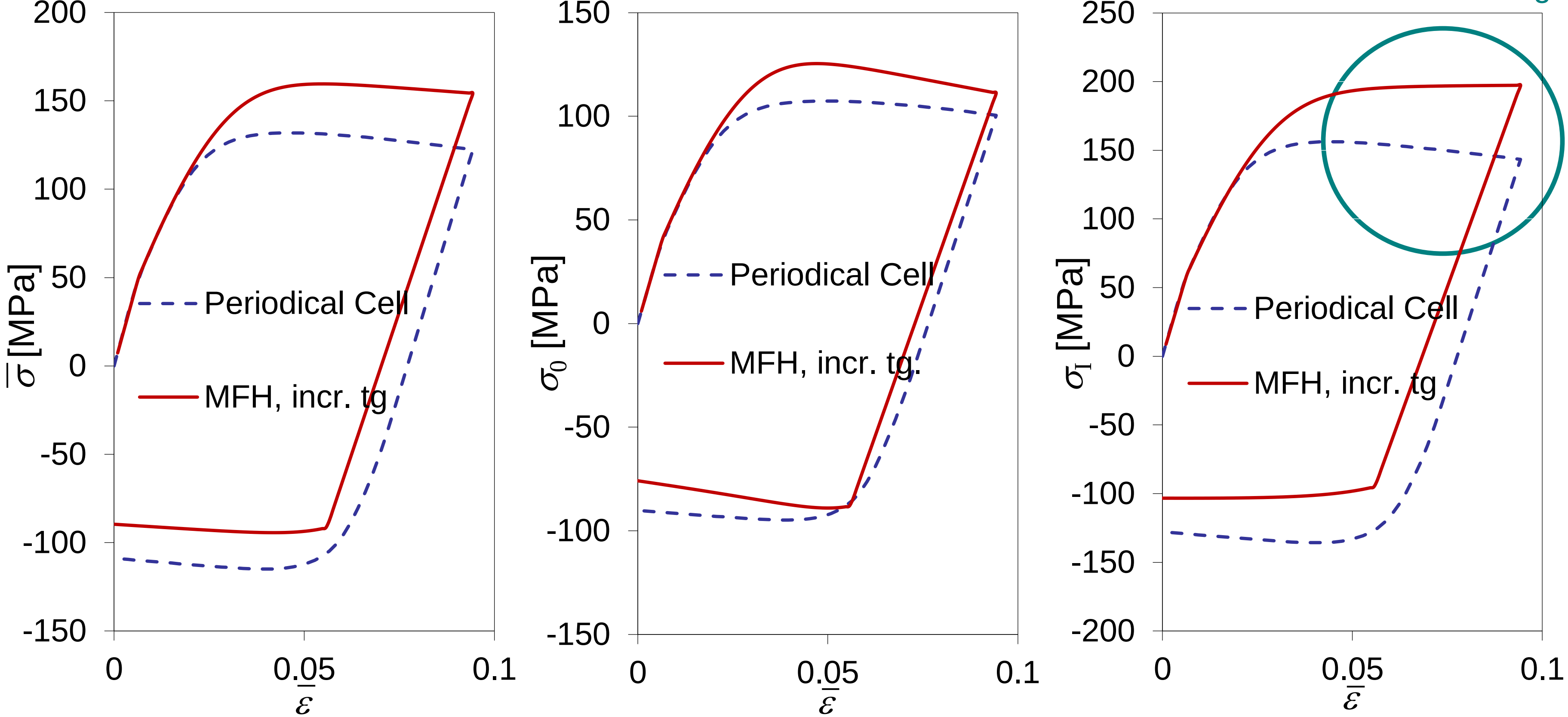
- Limitation of the method
  - Fictitious composite
    - 30%-UD fibres
    - 50%-UD fibres



  - Less accurate during softening for high fibres-volume-ratios

- Limitation of the method (2)
  - Fictitious composite
    - 50%-UD fibres
    - Analyse phases behaviours
  - Due to the incremental formalism, stress in fibres cannot decreases during loading

No fibres unloading

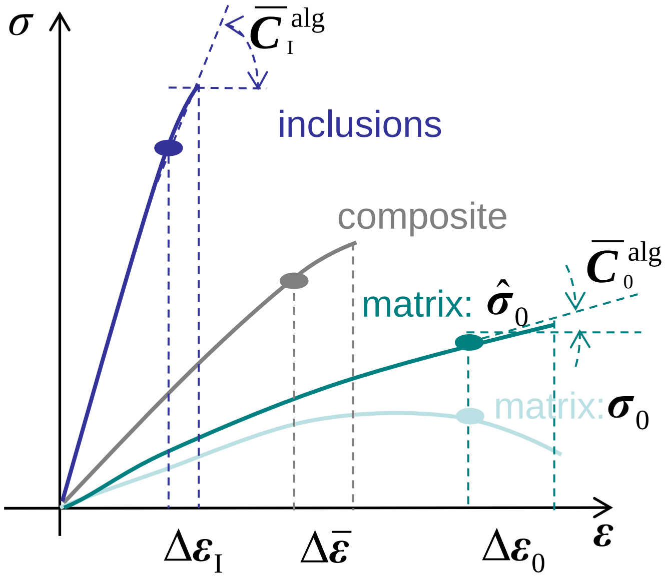


Non-local damage mean-field-homogenization

- Problem
  - We want the fibres to get unloaded during the matrix damaging process
    - For the incremental-tangent approach

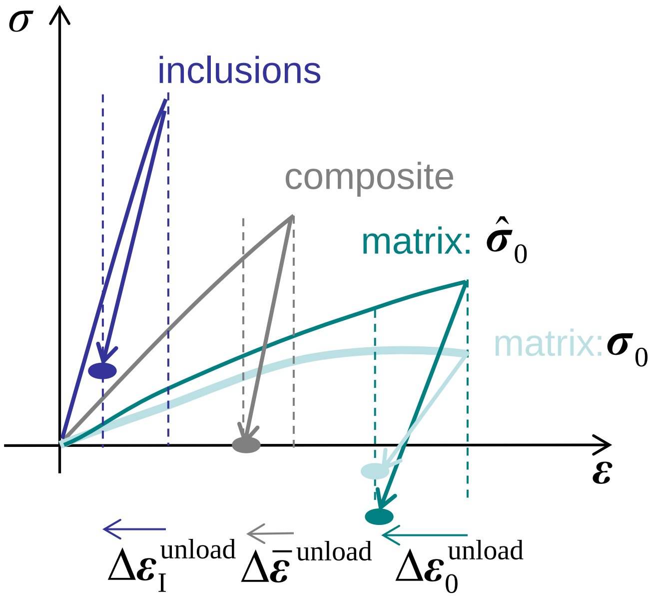
$$\Delta\boldsymbol{\varepsilon}_{\mathrm{I}} = \boldsymbol{B}^{\varepsilon}\left(\mathrm{I}, (1-D)\overline{\boldsymbol{C}}_{0}^{\mathrm{alg}}, \overline{\boldsymbol{C}}_{\mathrm{I}}^{\mathrm{alg}}\right) : \Delta\boldsymbol{\varepsilon}_{0}$$

    - To unload the fibres ($\boldsymbol{\varepsilon}_{\mathrm{I}} < 0$)with such approach would require $\overline{\boldsymbol{C}}_{\mathrm{I}}^{\mathrm{alg}} < 0$
    - We cannot use the incremental tangent MFH
  - We need to define the LCC from another stress state



Non-local damage mean-field-homogenization

- Idea
  - New incremental-secant approach
    - Perform a virtual elastic unloading from previous solution
      - Composite material unloaded to reach the stress-free state
      - Residual stress in components



Non-local damage mean-field-homogenization

- Idea
  - New incremental-secant approach
    - Perform a virtual elastic unloading from previous solution
      - Composite material unloaded to reach the stress-free state
      - Residual stress in components
    - Apply MFH from unloaded state
      - New strain increments (>0)

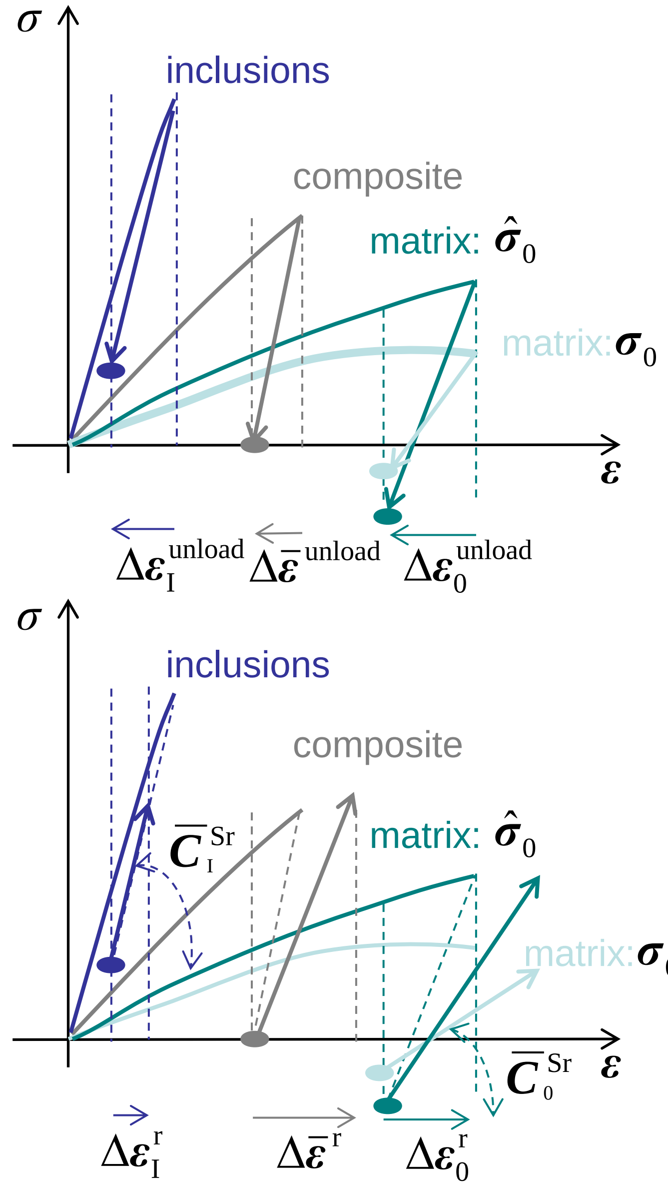
$$\Delta\boldsymbol{\varepsilon}^{\mathrm{r}}_{\mathrm{I}/0} = \Delta\boldsymbol{\varepsilon}_{\mathrm{I}/0} + \Delta\boldsymbol{\varepsilon}^{\mathrm{unload}}_{\mathrm{I}/0}$$

      - Use of secant operators

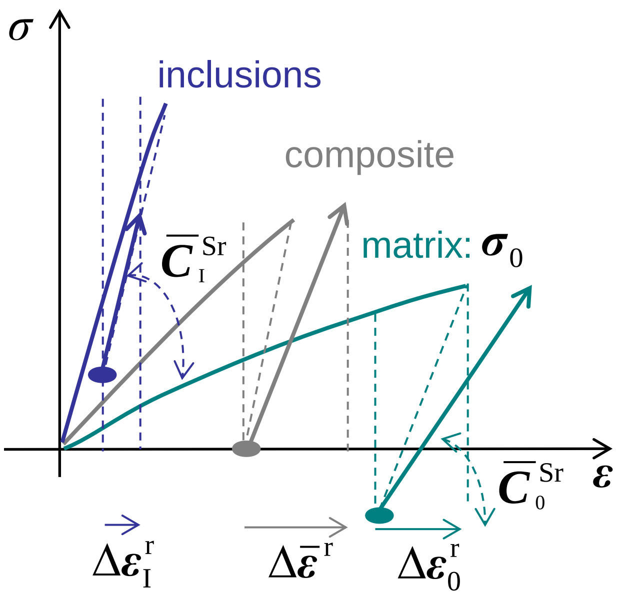
$$\Delta\boldsymbol{\varepsilon}^{\mathrm{r}}_{\mathrm{I}} = \boldsymbol{B}^{\varepsilon}\left(\mathrm{I}, (1-D)\overline{\boldsymbol{C}}^{\mathrm{Sr}}_{0}, \overline{\boldsymbol{C}}^{\mathrm{Sr}}_{\mathrm{I}}\right) : \Delta\boldsymbol{\varepsilon}^{\mathrm{r}}_{0}$$

      - Possibility of have unloading

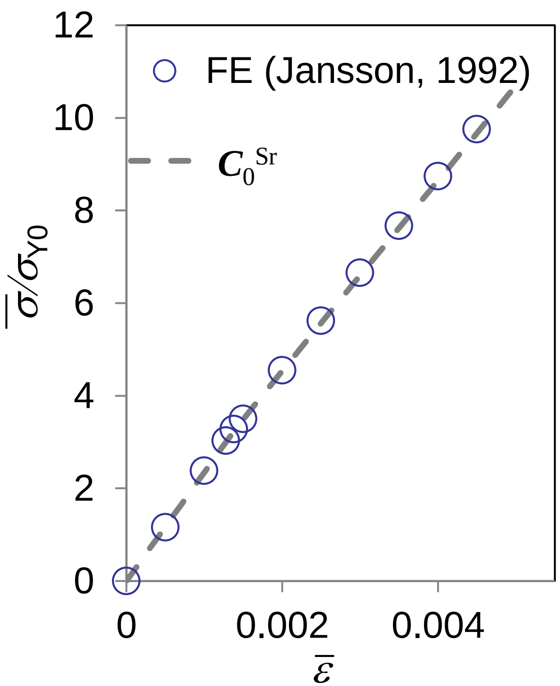
$$\begin{cases} \Delta\boldsymbol{\varepsilon}^{\mathrm{r}}_{\mathrm{I}} > 0 \\ \Delta\boldsymbol{\varepsilon}_{\mathrm{I}} < 0 \end{cases}$$



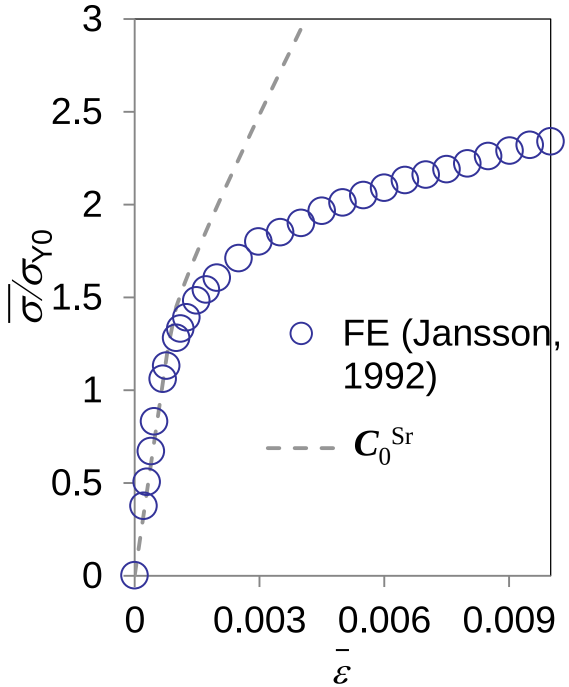
- Zero-incremental-secant method
  - Continuous fibres
    - 55 % volume fraction
    - Elastic
  - Elasto-plastic matrix
  - For inclusions with high hardening (elastic)
    - Model is too stiff



Longitudinal tension



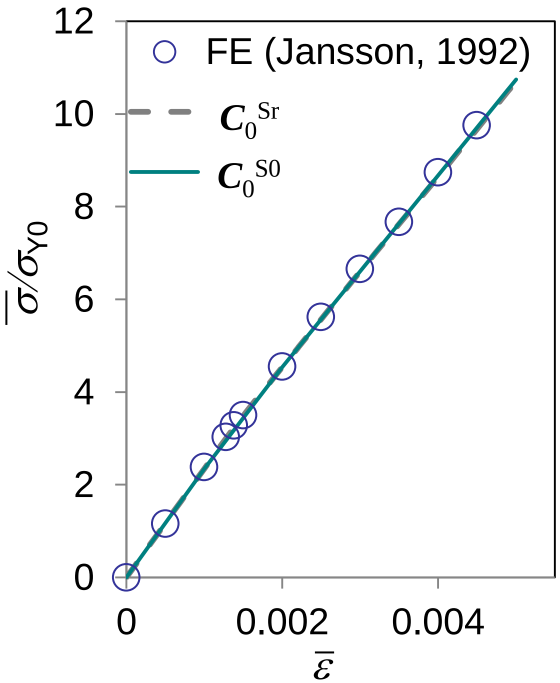
Transverse loading



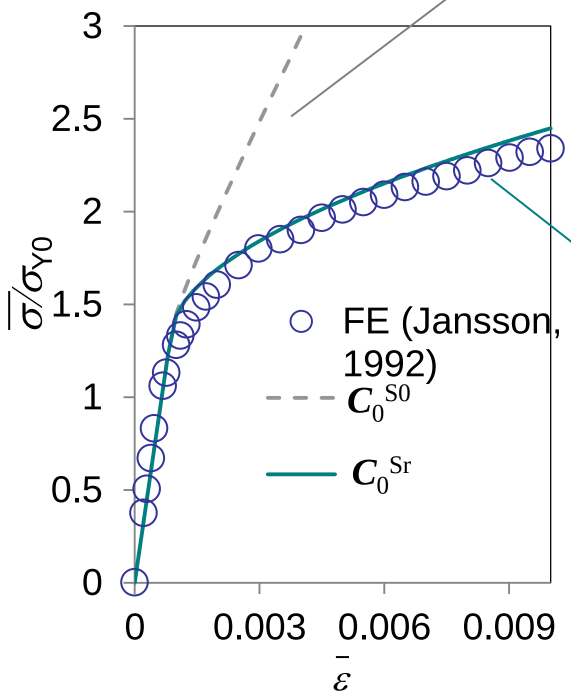
Non-local damage mean-field-homogenization

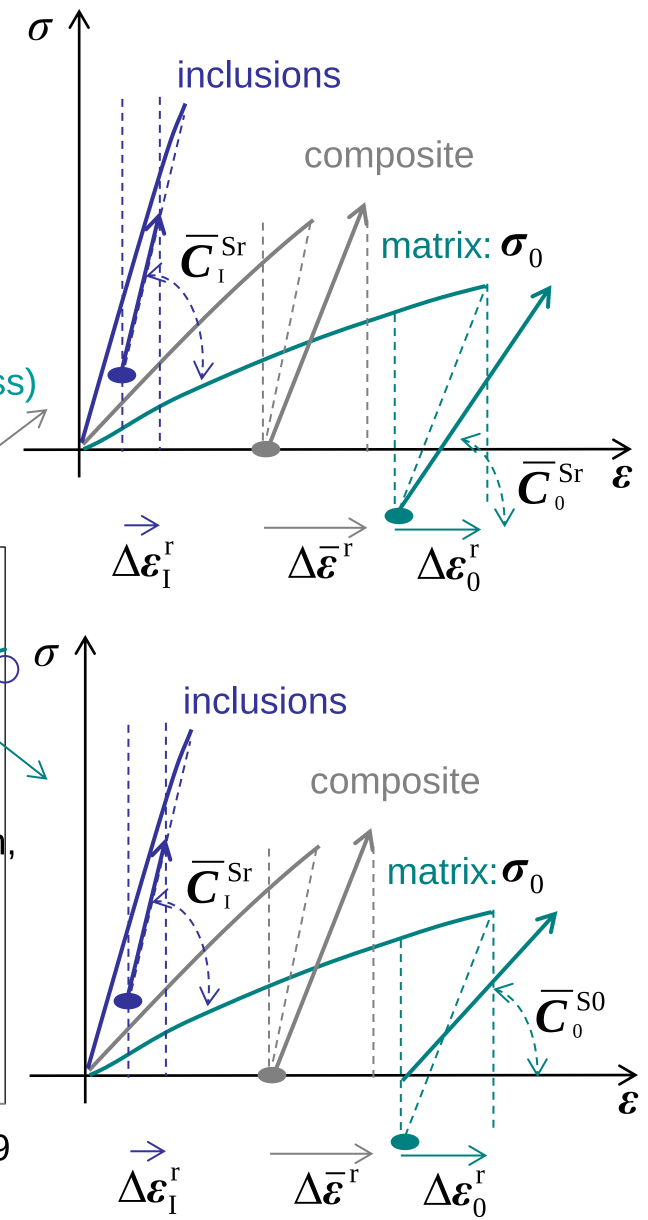
- Zero-incremental-secant method
  - Continuous fibres
    - 55 % volume fraction
    - Elastic
  - Elasto-plastic matrix
  - Secant model in the matrix
    - Modified if stiffer inclusions (negative residual stress)

Longitudinal tension



Transverse loading





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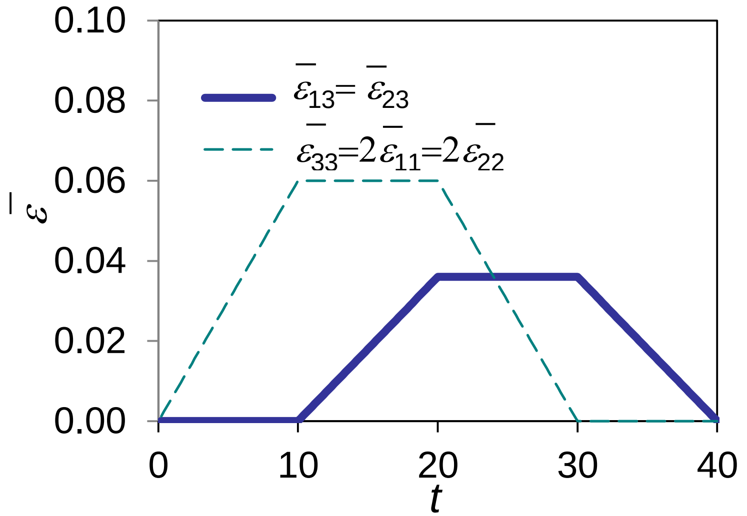
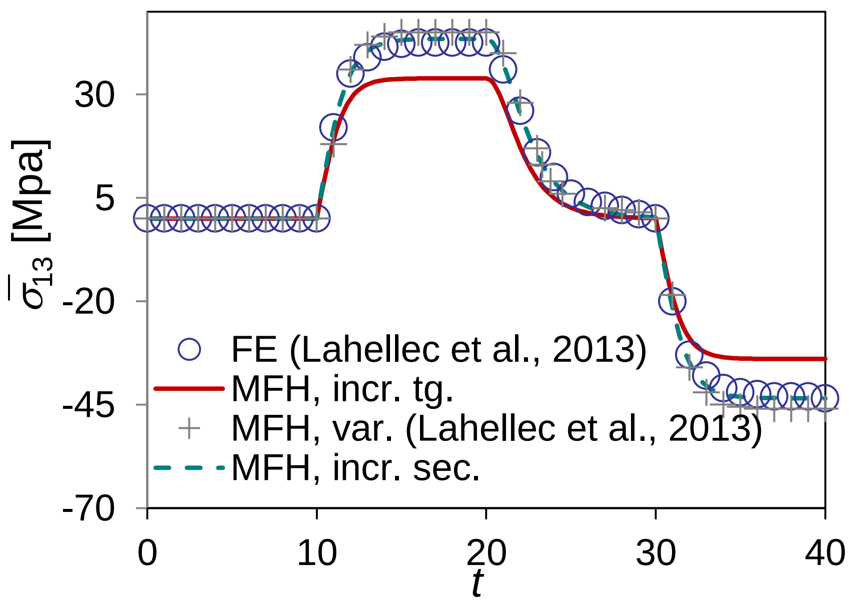
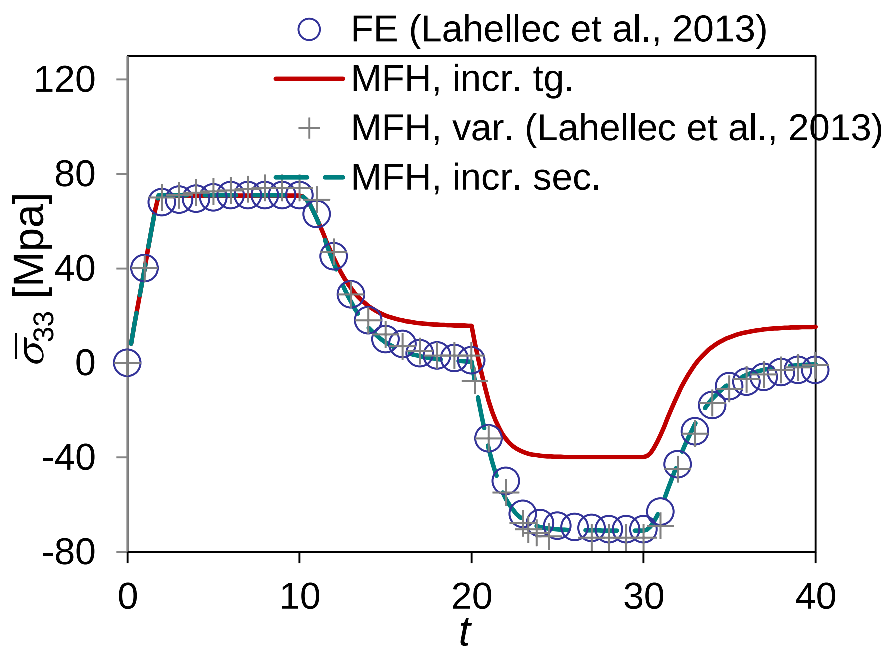
Non-local damage mean-field-homogenization

- Verification of the method
  - Spherical inclusions
    - 17 % volume fraction
    - Elastic
  - Elastic-perfectly-plastic matrix
  - Non-radial loading

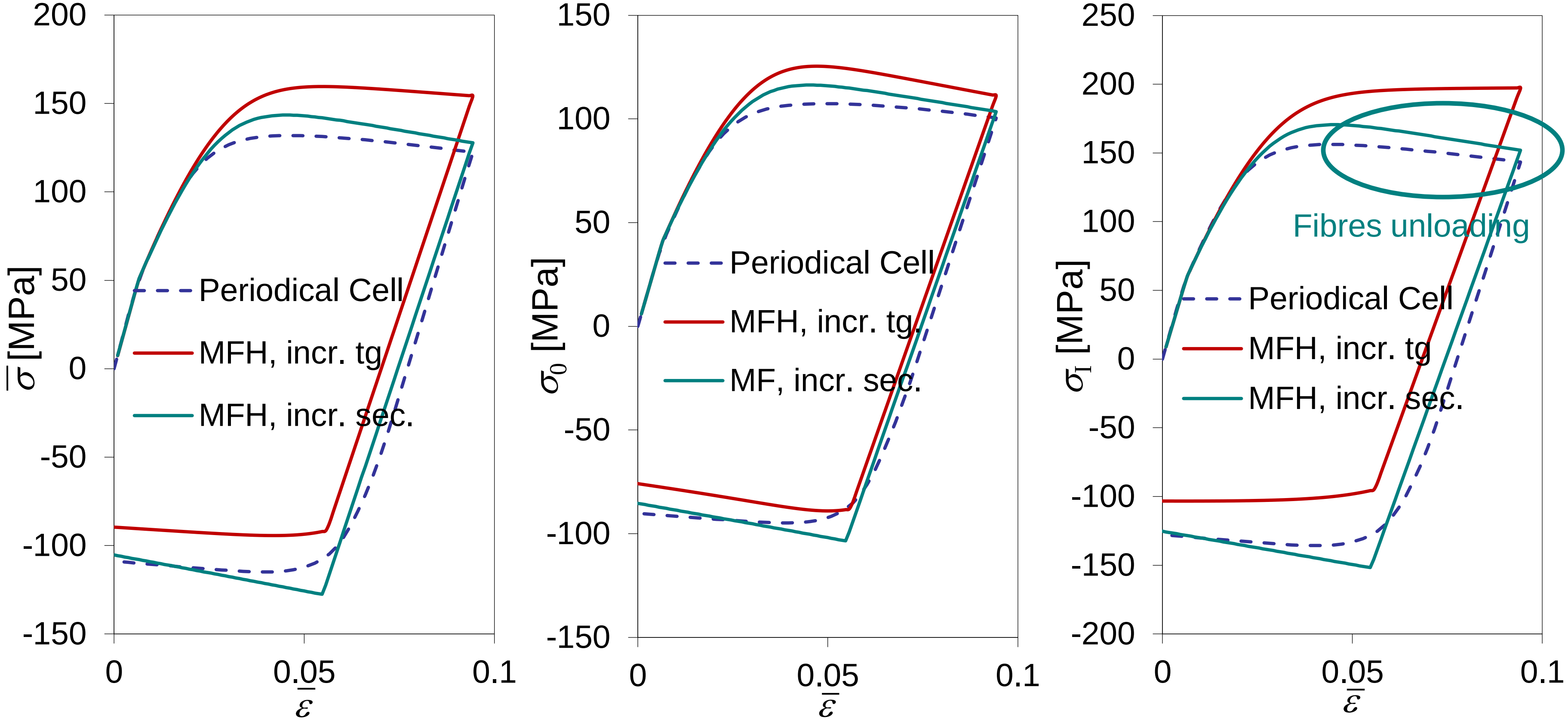






Non-local damage mean-field-homogenization

- New results for damage
  - Fictitious composite
    - 50%-UD fibres
    - Analyse phases behaviours



Conclusions

- Multi-scale methods
  - Allows considering
    - Micro-structure geometry
    - Non-linear behaviours of the micro-constituents
  - Rely on different techniques
    - Computational
    - MFH
    - …
  - Accuracy depends
    - On the model
    - On the micro-structure complexity
    - …

- Non-local damage-enhanced MFH
  - Good description of the meso-scale response
  - Can be used to study coupons problems