Multiscale Simulations of Composites with Non-Local Damage-Enhanced Mean-Field Homogenization

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/Outline

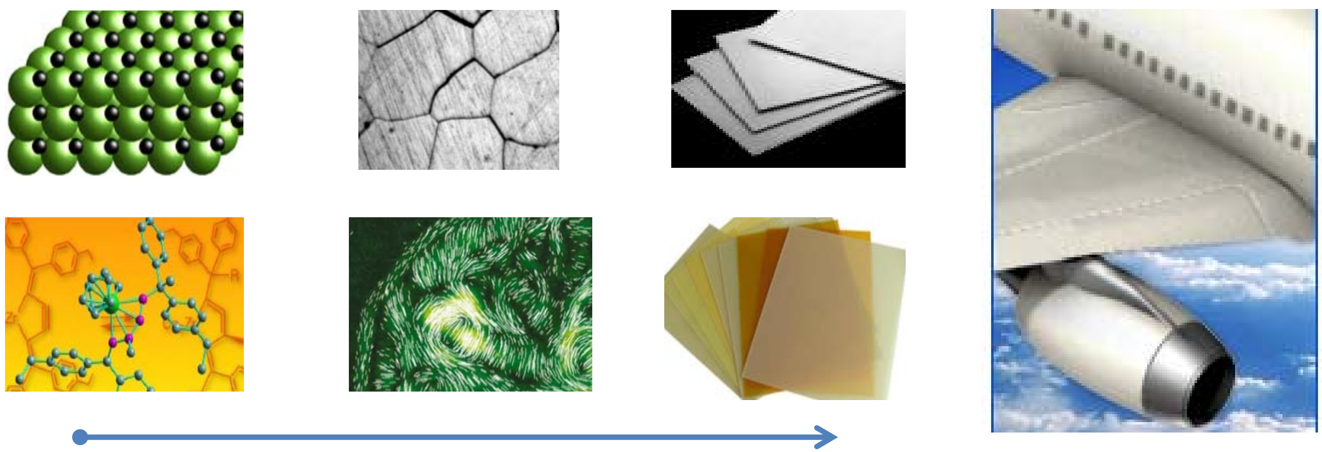
- Introduction
- Mean Field Homogenization
- Nonlocal Approach and Implicit Gradient Formulation
- Ductile Damage in the Matrix of Composite
- Finite Element Implementation
- Validation and Simulation

Why Multiscale?

- Materials are multiscale in nature:

Metals

Polymers



10^{-9} m — 1 m

Molecular Dynamics

Monte Carlo Method, Statistical Mechanics …

Continuum Mechanics

/Introduction

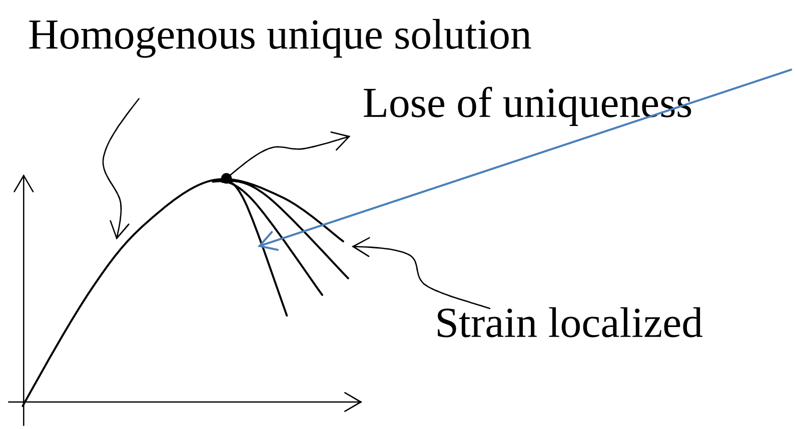
Why Multiscale?

- Multiscale Methods for Composites
  - ❖ For material design:
    These effective properties are difficult or expensive to measure.
  - ❖ For composite structures analysis:
    - Continuum mechanics analysis at Macroscale
      Accuracy!
    - Take into account the individual component properties and geometrical arrangements.
      Expensive, unreachable!
- Solution:
  - ❖ The engineering problems are solved at macroscopic scale with the homogenized properties.
  - ❖ The homogenized properties are obtained from the individual component properties and their microstructure.

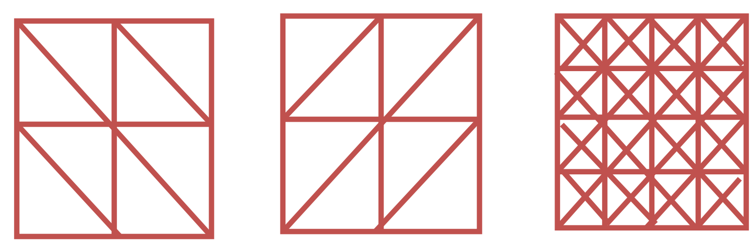
/Introduction

Problem in finite element simulations

- 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

/Introduction

Problem in finite element simulations

Multiscale Methods have this problem too!

- Solution:

  Introduce high order term in the continuum description

  Strain gradient model, nonlocal model…

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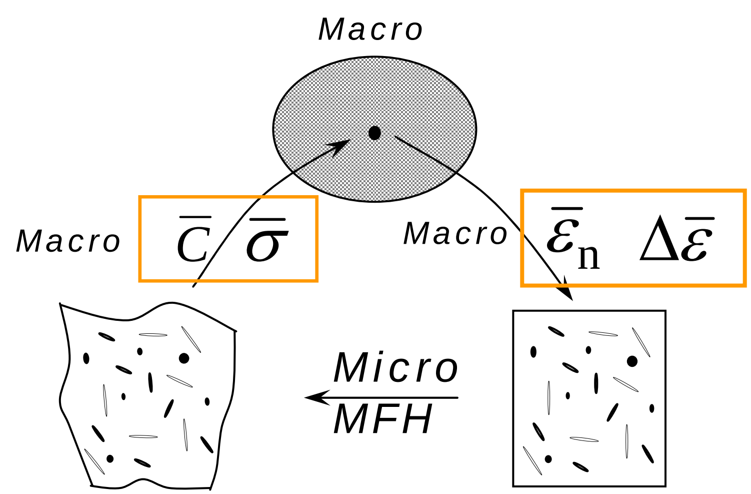
/Mean Field Homogenization

- At the macroscale, the problem is a classical continuum mechanics problem (Finite Element method).
- At a macroscopic material point the properties of the material correspond to a representative volume element (RVE) of the microstructure.

Basing on
The marco strain $\bar{\varepsilon}$ and stress $\bar{\sigma}$ equal the average strain $\langle \varepsilon \rangle$ and stress $\langle \boldsymbol{\sigma} \rangle$ over a RVE

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



/Mean Field Homogenization

- How to get $\overline{C}$ in RVE? Such that $\langle \boldsymbol{\sigma} \rangle = \overline{\boldsymbol{C}} : \langle \boldsymbol{\varepsilon} \rangle$
  - Direct finite element simulation
  - Semi-analytical mean field homogenization models

(Voigt, Reuss, **Mori-Tanaka**, Double-Inclusion, Self-Consistent …)

- Two-phase composite
  - Volume fraction $v_0 + v_1 = 1$

$$\langle \boldsymbol{\sigma} \rangle = v_0 \langle \boldsymbol{\sigma} \rangle_{\omega_0} + v_1 \langle \boldsymbol{\sigma} \rangle_{\omega_1}$$

$$\langle \boldsymbol{\varepsilon} \rangle = v_0 \langle \boldsymbol{\varepsilon} \rangle_{\omega_0} + v_1 \langle \boldsymbol{\varepsilon} \rangle_{\omega_1}$$

$$\langle \boldsymbol{\sigma} \rangle_{\omega_1} = \overline{\boldsymbol{C}}_1 : \langle \boldsymbol{\varepsilon} \rangle_{\omega_1}$$

$$\langle \boldsymbol{\sigma} \rangle_{\omega_0} = \overline{\boldsymbol{C}}_0 : \langle \boldsymbol{\varepsilon} \rangle_{\omega_0}$$

???

$$\langle \varepsilon \rangle_{\omega_1} = B^{\varepsilon} : \langle \varepsilon \rangle_{\omega_0}$$

Subscription: 0(matrix) and 1(inclusion)

/Mean Field Homogenization

- Single inclusion problem

$$\langle \varepsilon \rangle_{\omega_1} = H^{\varepsilon}(I, \overline{C}_0, \overline{C}_1) : \varepsilon^{\infty}$$

H^{ε} is single inclusion strain concentration tensor (numerical, analytical)

$$H^{\varepsilon} = [I + S : \overline{C}_0^{-1} : (\overline{C}_1 - \overline{C}_0)]^{-1}$$

S is Eshelby's tensor

- Multiple inclusion problem

$$\langle \varepsilon \rangle_{\omega_1} = B^{\varepsilon} : \langle \varepsilon \rangle_{\omega_0} \qquad \langle \varepsilon \rangle_{\omega_1} = A^{\varepsilon} : \langle \varepsilon \rangle$$

Mori-Tanaka model:

$$\varepsilon^{\infty} = \langle \varepsilon \rangle_{\omega_0} \quad \text{and} \quad B^{\varepsilon} = H^{\varepsilon}$$

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/Nonlocal Approach

- Description

Some variables (a) are replaced by their <u>weighted (ϕ) average</u> over a characteristic volume (Vc) to <u>reflect the interaction between neighboring material points.</u>

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

The state variable a can be strains, internal variables (eg. accumulated plastic strain, damage….)

Problem: Weight function w ?? Characteristic volume Vc ??

/Implicit Gradient Formulation

- Implicit gradient formulation *:
  - ❖ Green's function $G(\boldsymbol{y};\boldsymbol{x})$ → weight function $w(\boldsymbol{y};\boldsymbol{x})$

$$\tilde{a}(\boldsymbol{X}) = \frac{1}{V_C}\int_{V_C} a(\boldsymbol{y})\phi(\boldsymbol{y};\boldsymbol{X})\mathrm{d}V \longrightarrow \tilde{a}(\boldsymbol{X}) - l^2\nabla^2\tilde{a} = a(\boldsymbol{X})$$

  - ❖ The natural boundary condition: $\dfrac{\partial\tilde{a}}{\partial n} = n_i\dfrac{\partial\tilde{a}}{\partial X_i} = 0$

/Implicit Gradient Formulation

- Composites are anisotropic at the ply scale
  - ❖ Characteristic size should depend on the direction

$$\tilde{a}(\boldsymbol{X}) - l^2 \nabla^2 \tilde{a} = a(\boldsymbol{X}) \quad \longrightarrow \quad \tilde{a} - \nabla \cdot (\boldsymbol{c}_{\mathrm{g}} \cdot \nabla \tilde{a}) = a$$

  - ❖ The natural boundary condition becomes:

$$(\boldsymbol{c}_{\mathrm{g}} \cdot \nabla \tilde{a}) \cdot \boldsymbol{n} = 0$$

* Peerlings et al., 1996

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/Ductile Damage in the Matrix of Composite

- Damage in matrix only (neglect the Damage in fiber)
- Lemaitre - Chaboche ductile damage model:

$$\dot{D} = (\frac{Y}{S_0})^n \dot{p}$$

where S_0 and n are the material parameters

Y is the strain energy release rate $Y = \frac{1}{2}\boldsymbol{\varepsilon}^{\mathrm{e}} : \boldsymbol{E}_0 : \boldsymbol{\varepsilon}^{\mathrm{e}}$

p is the accumulated plastic strain $\dot{p} = [\frac{2}{3}\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} : \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}]^{1/2}$, $p = \int \dot{p}\mathrm{d}t$

- Nonlocal damage:

$$\dot{D} = \begin{cases} 0, & \text{if } \tilde{p} \leqslant p_C \\ (\frac{Y}{S_0})^s \dot{\tilde{p}}, & \text{if } \tilde{p} > p_C \end{cases} \qquad \tilde{p} - \nabla \cdot (\boldsymbol{c}_{\mathrm{g}} \cdot \nabla \tilde{p}) = p$$

/Ductile Damage in the Matrix of Composite

- Considering the damage in matrix, the incremental form of stress in composite*:

$$\delta\bar{\boldsymbol{\sigma}} = v_0\delta\boldsymbol{\sigma}_0 + v_{\mathrm{I}}\delta\boldsymbol{\sigma}_{\mathrm{I}} \qquad \hat{\boldsymbol{\sigma}}_0 = \boldsymbol{\sigma}_0/(1-D)$$

$$\rightarrow \delta\bar{\boldsymbol{\sigma}} = \underbrace{v_{\mathrm{I}}\bar{\boldsymbol{C}}_{\mathrm{I}}^{\mathrm{alg}} : \delta\boldsymbol{\varepsilon}_{\mathrm{I}} + v_0\bar{\boldsymbol{C}}_0^{\mathrm{algD}} : \delta\boldsymbol{\varepsilon}_0}_{\text{Mori-Tanaka}} - v_0\left(\hat{\boldsymbol{\sigma}}_0 \otimes \frac{\partial D}{\partial \boldsymbol{\varepsilon}_0}\right) : \delta\boldsymbol{\varepsilon}_0 - v_0\hat{\boldsymbol{\sigma}}_0\frac{\partial D}{\partial \tilde{p}}\delta\tilde{p}$$

$$\delta\bar{\boldsymbol{\sigma}} = \left[\bar{\boldsymbol{C}}^{\mathrm{algD}} - v_0\left(\hat{\boldsymbol{\sigma}}_0 \otimes \frac{\partial D}{\partial \boldsymbol{\varepsilon}_0}\right) : \frac{\partial \boldsymbol{\varepsilon}_0}{\partial \bar{\boldsymbol{\varepsilon}}}\right] : \delta\bar{\boldsymbol{\varepsilon}} + \left[\boldsymbol{C}^{\tilde{p}} - v_0\left(\hat{\boldsymbol{\sigma}}_0 \otimes \frac{\partial D}{\partial \boldsymbol{\varepsilon}_0}\right) : \frac{\partial \boldsymbol{\varepsilon}_0}{\partial \tilde{p}} - v_0\hat{\boldsymbol{\sigma}}_0\frac{\partial D}{\partial \tilde{p}}\right]\delta\tilde{p}$$

Subscription: 0(matrix) and I(inclusion)

* Doghri I. et al., 2003

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Governing equations

- For implicit gradient enhanced elastic-plasticity

$$0 = \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}^T + \rho \boldsymbol{f} \quad \text{in composite}$$

$$\tilde{p} - \nabla \cdot (\boldsymbol{c}_{\mathrm{g}} \cdot \nabla \tilde{p}) = p \quad \text{in matrix only}$$

- Discretization (in each element)

$$\tilde{p} = \boldsymbol{N}_{\tilde{p}} \tilde{\boldsymbol{p}}$$

$$\boldsymbol{U} = \boldsymbol{N}_u \boldsymbol{u}$$

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

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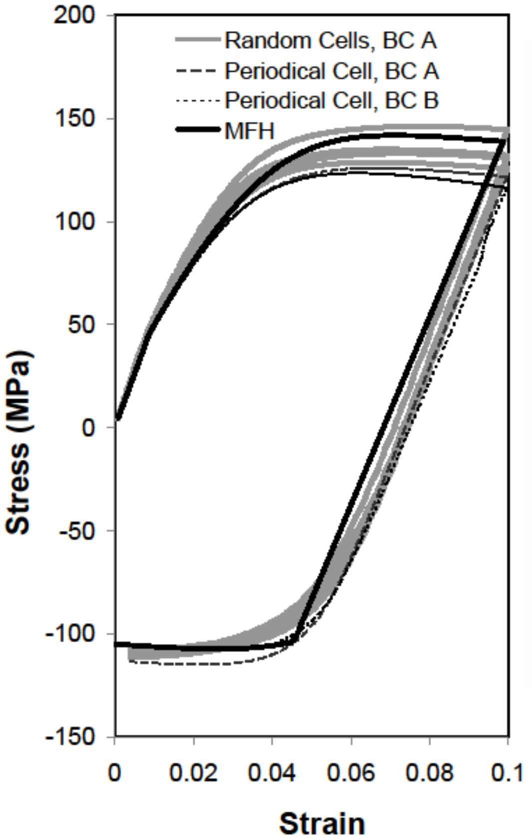
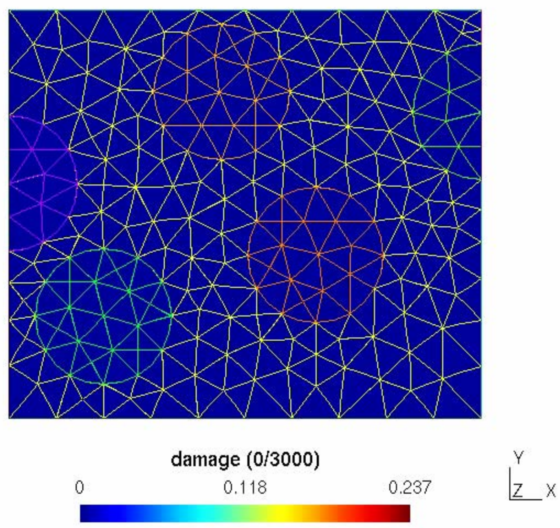
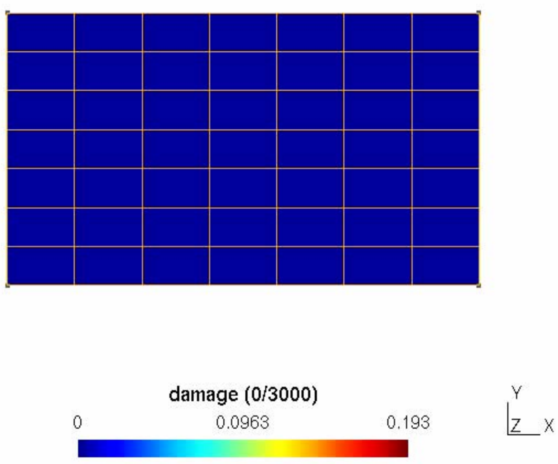
/Validation and Simulation

Validation: DNS vs. FE/MFH

- Epoxy-CF (30%)







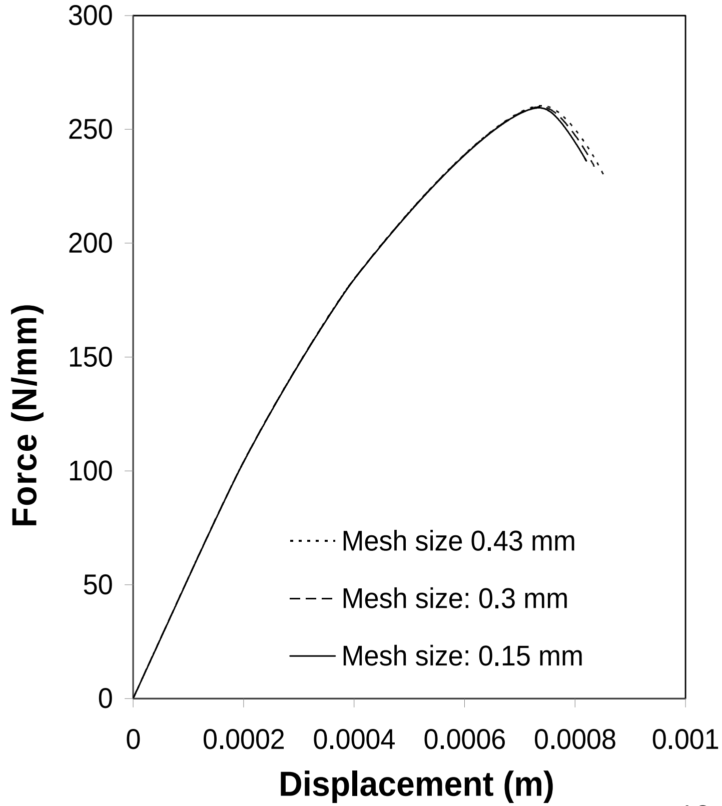
/Validation and Simulation

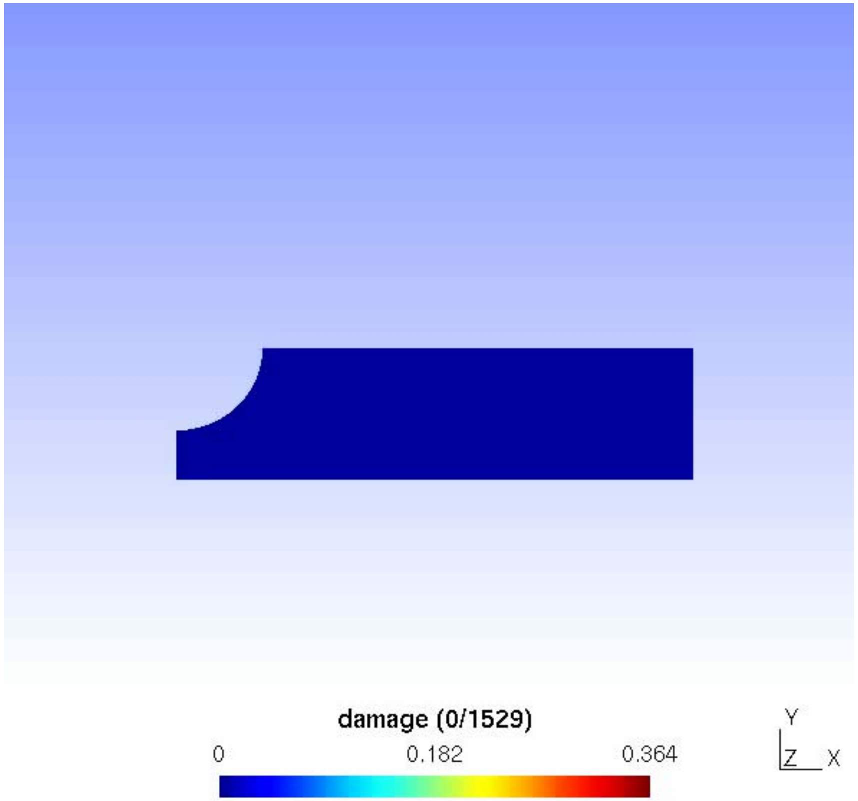
Simulation

- Notched ply

Epoxy-CF (30%), Transverse loading, single ply

Mesh independent

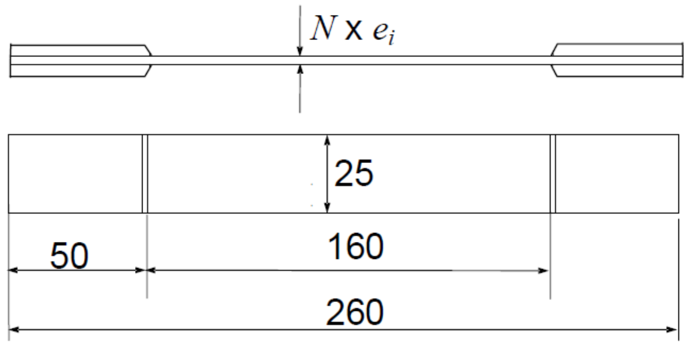


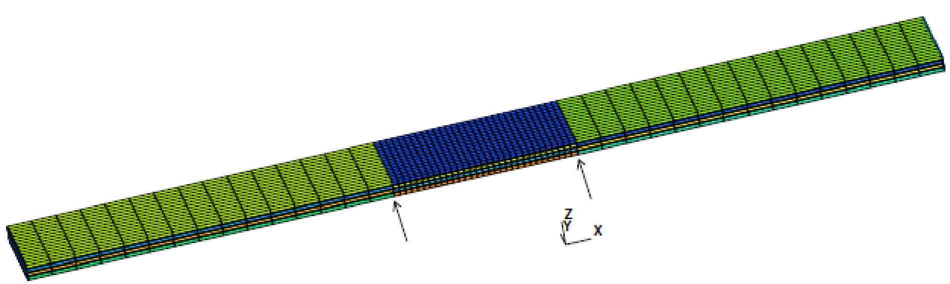


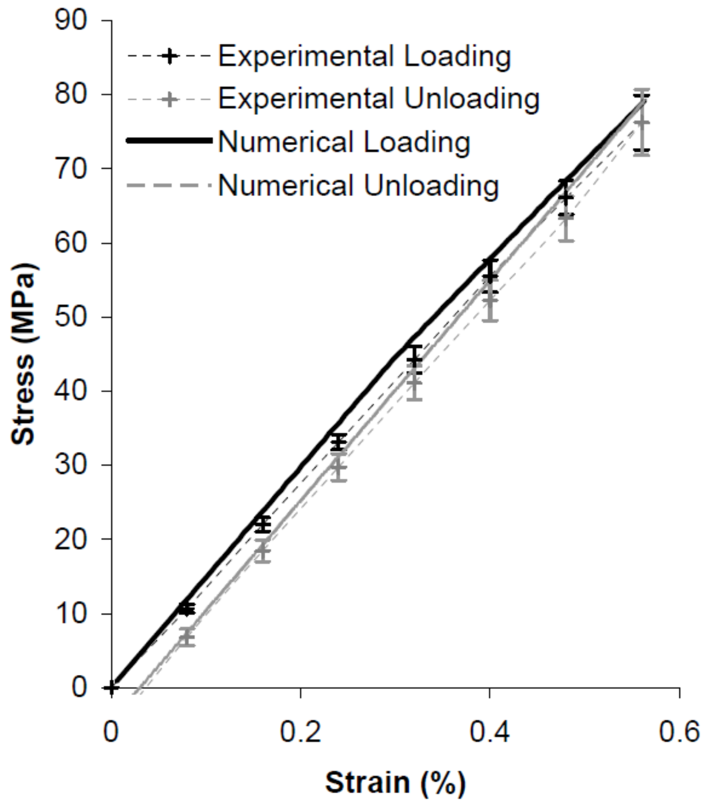
/Validation and Simulation

Comparison with experiments

- Tensile tests with unloading
  Epoxy-CF (60%), in plane loading, [-45/45/45/-45]



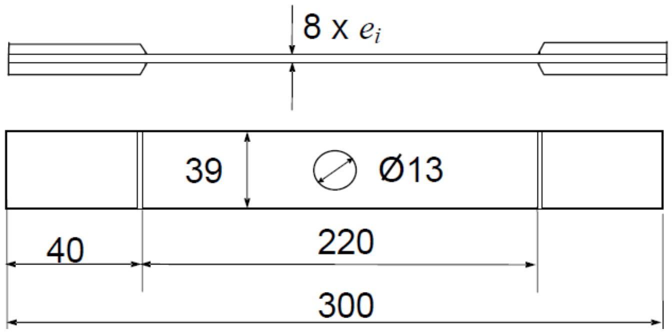


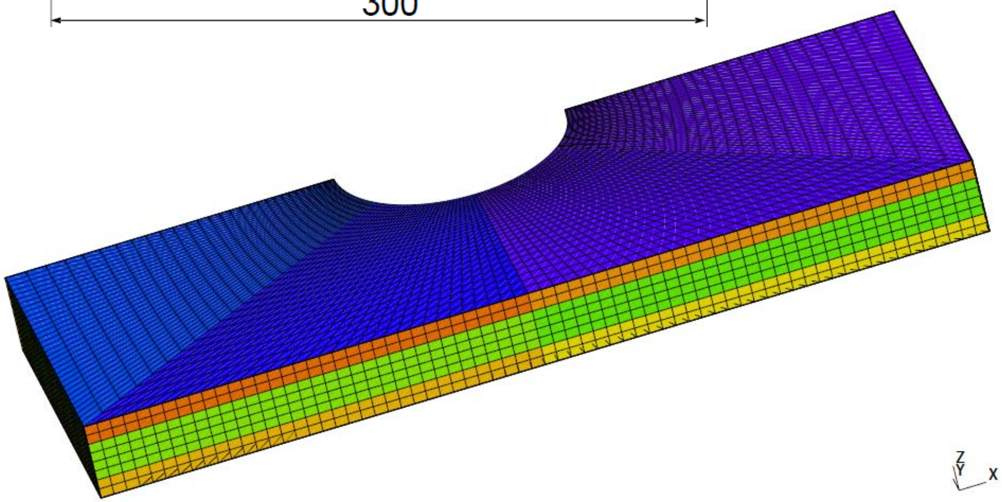


/Validation and Simulation

Comparison with experiments

- Tensile on open hole specimen
  Epoxy-CF (60%), in plane loading, [-45/45/45/-45]





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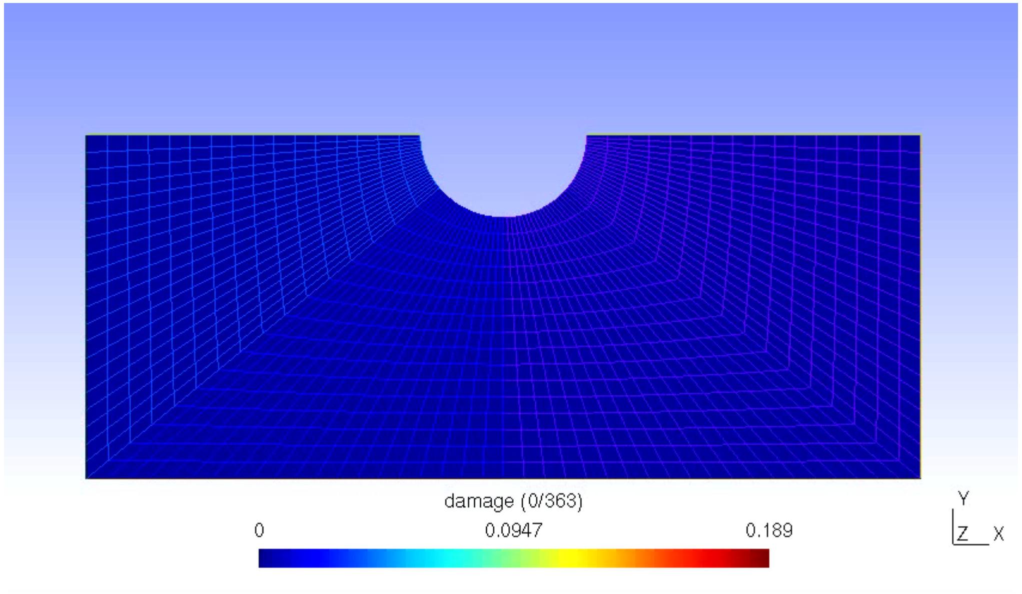

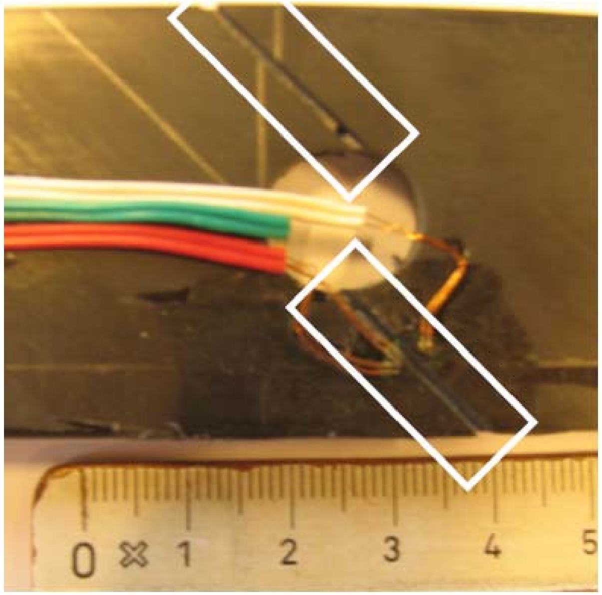

Thank you!

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