A multiscale computational homogenization method based on a hybrid discontinuous Galerkin formulation/ extrinsic cohesive zone model

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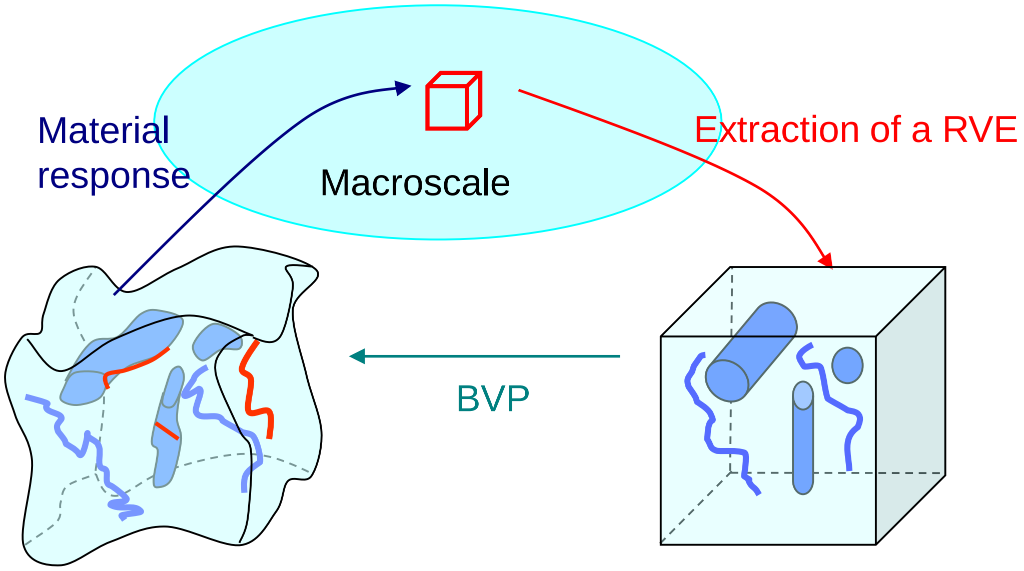
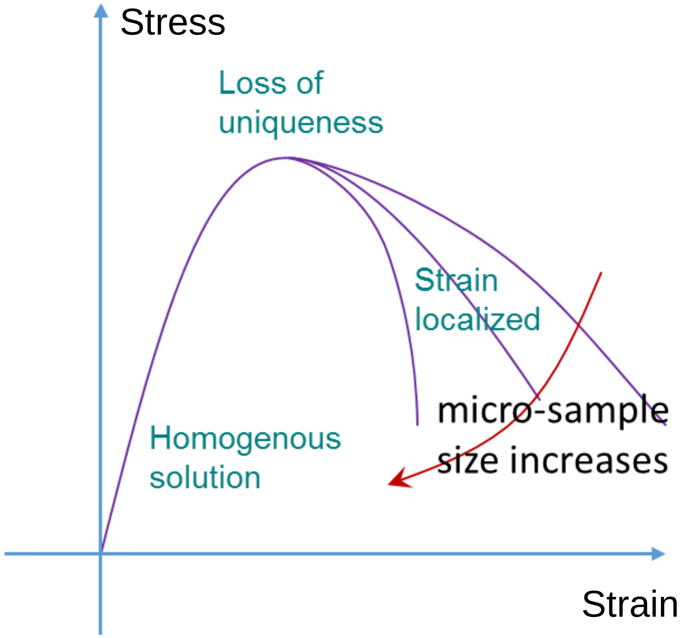
Introduction

- Computational homogenization (so-called FE^2) for micro-structured materials
  - Representative volume elements (RVE) are extracted from material microstructure
  - Two boundary value problems (BVP) are concurrently solved
    - Macroscale BVP
    - Microscale BVP defined on RVE with an appropriate boundary condition
  - Separation of length scales $L_{\mathrm{macro}} \gg L_{\mathrm{RVE}} \gg L_{\mathrm{micro}}$



Introduction

- FE^2 for microstructured materials with strain localization at the microscale
  - Homogenized stress/strain behavior involves softening part
  - Scale separation assumption can not be satisfied
  - Homogenized properties are not objective with respect to micro-sample sizes



- FE^2 for microstructured materials with strain localization at the microscale
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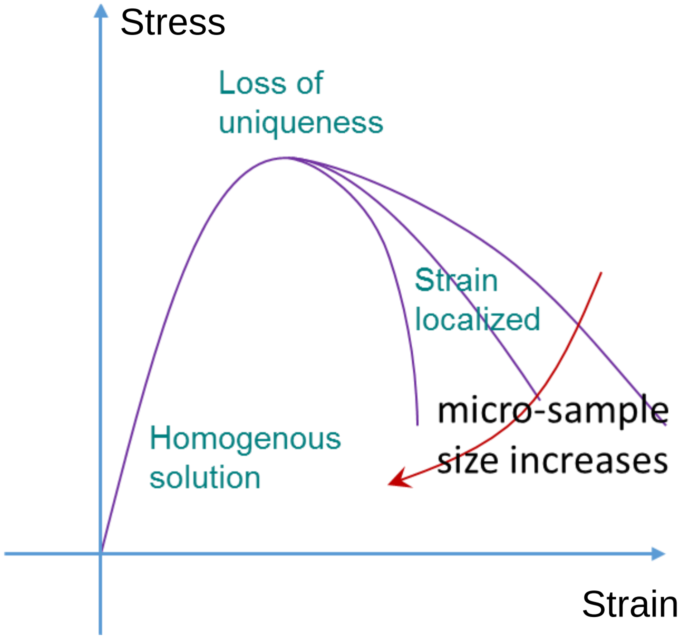


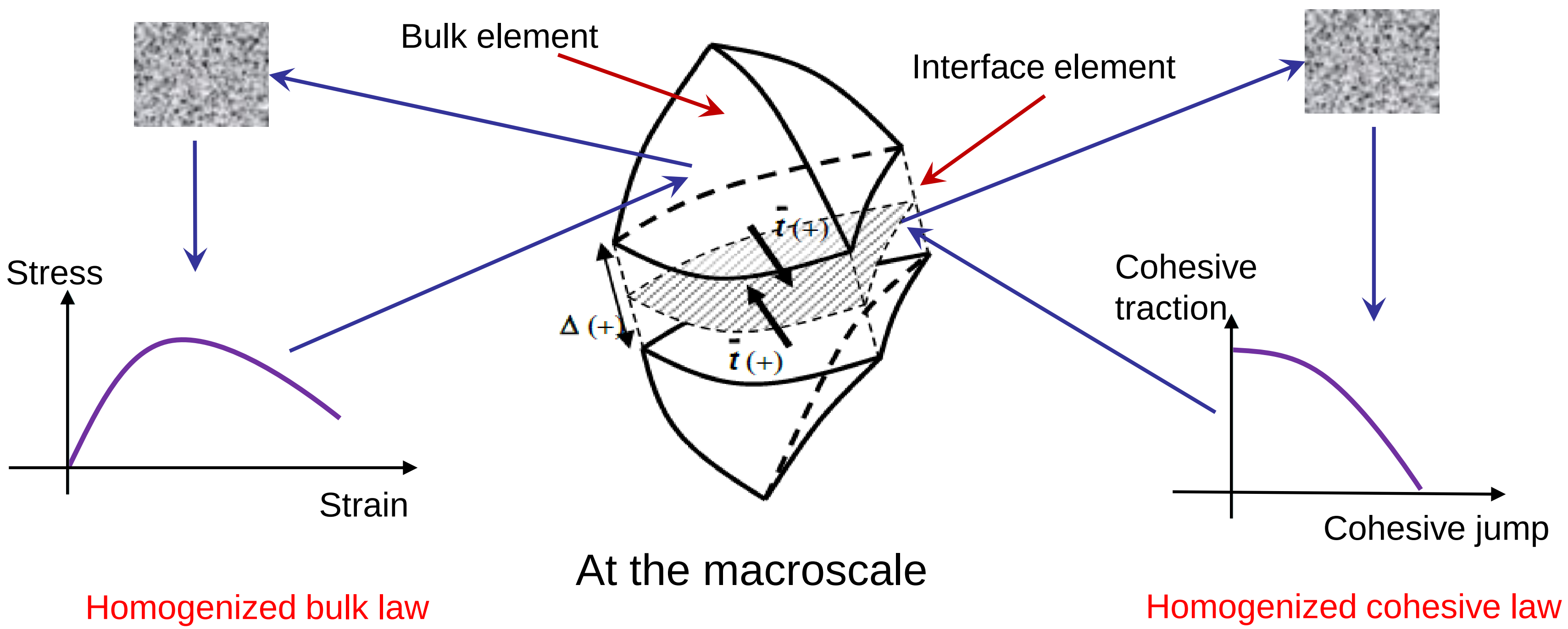
→Solution: FE^2 with enhanced discontinuity

  - Macroscale cohesive crack is inserted after onset of microscopic strain localization

(Nguyen V.-P. et al. CMAME 2010, Coenen E. et al. JMPS 2012)

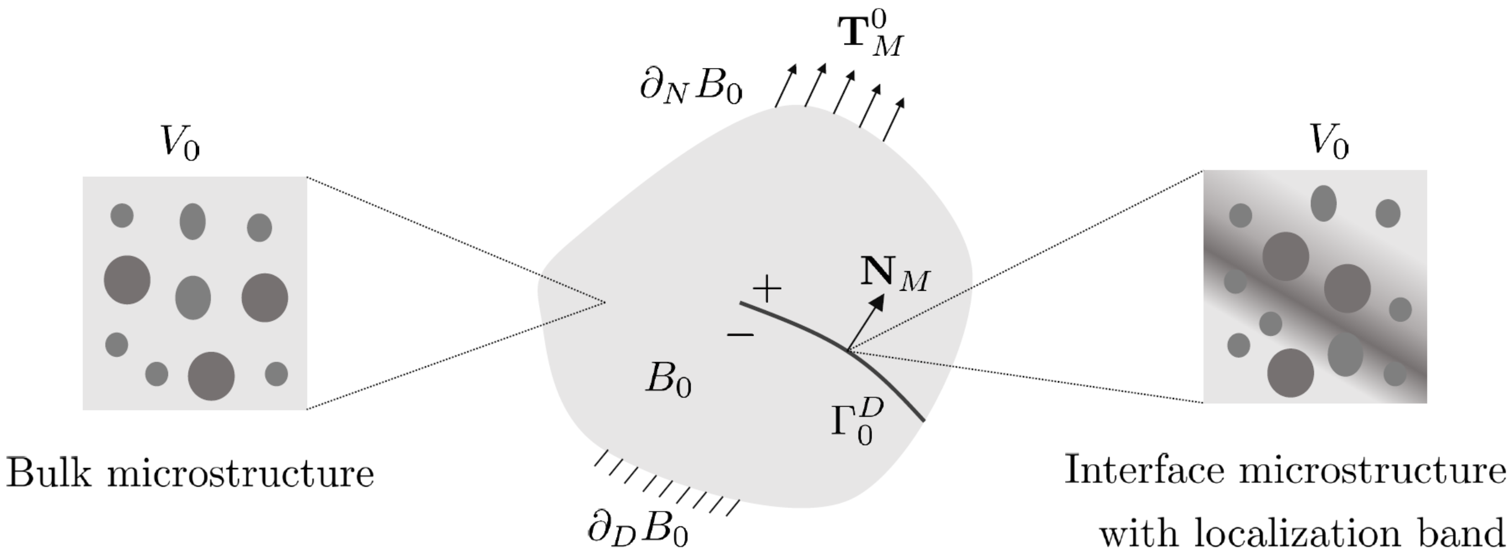
Computational strategy

- FE^2 with enhanced discontinuity based on a hybrid Discontinuous-Galerkin/ Extrinsic cohesive zone model (DG/CZM) formulation
  - Prior to the microscopic strain localization:
    - FE^2 based on DG formulation (Nguyen V.-D. et al. CMAME 2013)
  - After the onset of microscopic strain localization:
    - FE^2 based on DG/CZM formulation
    - Cohesive crack is inserted after onset of microscopic localization



Content

- Multiscale statement
- DG formulation
- Hybrid DG/CZM formulation
- Numerical examples



- Macroscopic boundary value problem
  - Bulk part

$$\begin{cases} \mathbf{P}_M \cdot \boldsymbol{\nabla}_0 + \mathbf{B} = \mathbf{0} \text{ on } B_0 \\ \mathbf{u}_M = \mathbf{u}_M^0 \text{ on } \partial_D B_0 \\ \mathbf{P}_M \cdot \mathbf{N}_M = \mathbf{T}_M^0 \text{ on } \partial_N B_0 \end{cases}$$

  - Discontinuity

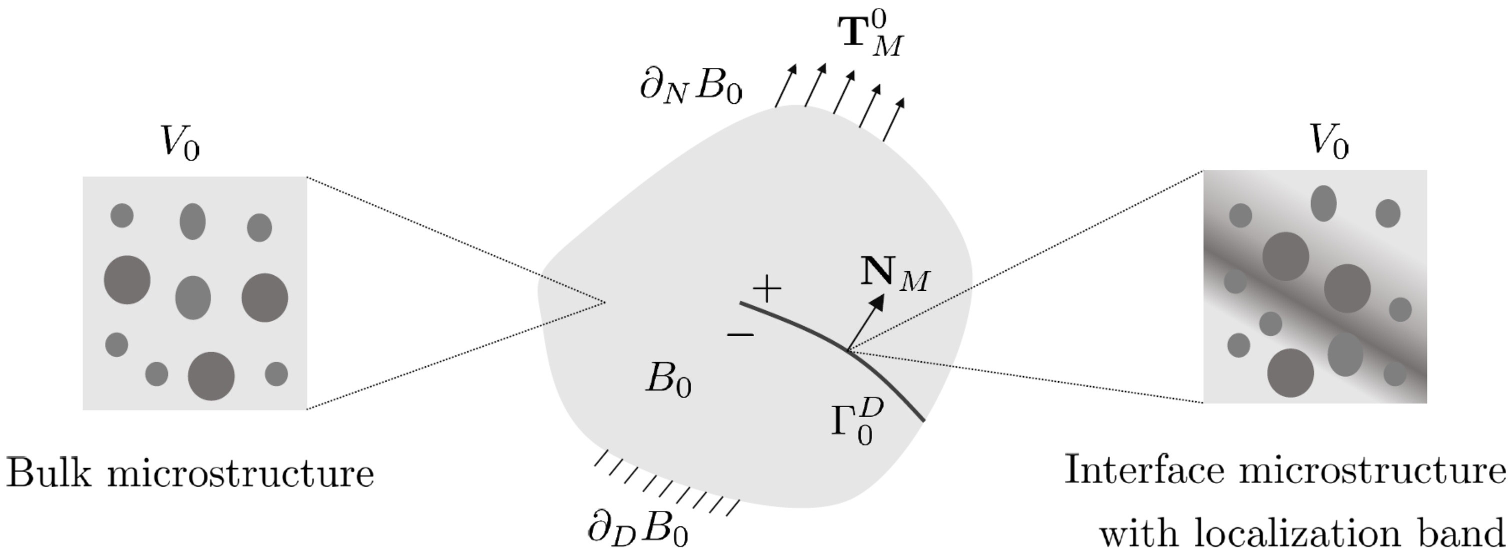
$$\begin{cases} [\![\mathbf{P}_M]\!] \cdot \mathbf{N}_M = \mathbf{0} \\ \langle \mathbf{P}_M \rangle \cdot \mathbf{N}_M = \mathbf{T}_M \end{cases} \quad \text{on } \Gamma_0^D$$

Jump operator $[\![\bullet]\!] = \bullet^+ - \bullet^-$

Mean operator $\langle \bullet \rangle = \frac{1}{2}\left(\bullet^+ + \bullet^-\right)$

$\mathbf{T}_M$: cohesive traction

Multiscale problem



- Microscopic boundary value problem
  - Implicit gradient enhanced nonlocal model

$$\begin{cases} \mathbf{P}_m \cdot \boldsymbol{\nabla}_0 = \mathbf{0} \\ \bar{\varphi} - c\Delta\bar{\varphi} = \varphi \end{cases} \quad \text{on } V_0$$

  - Microscopic constitutive laws are known

$$\begin{cases} \mathbf{P}_m & = (1-D)\hat{\mathbf{P}}_m \\ D & = D\left(\bar{\varphi}, \mathbf{F}_m, \mathbf{Q}\right) \\ \hat{\mathbf{P}}_m & = \hat{\mathbf{P}}_m\left(\mathbf{F}_m, \mathbf{Q}\right) \end{cases}$$

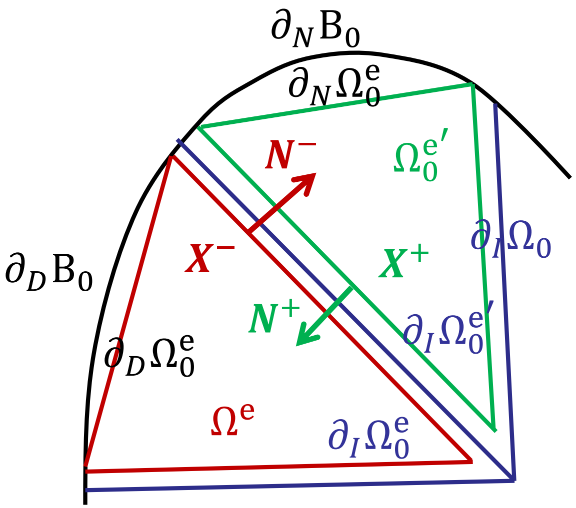
c : square of nonlocal length scale

$\mathbf{Q}$: internal variable

Discontinuous Galerkin formulation

- Weak form of the macroscopic BVP is obtained by applying integration by parts on each element Ω_0^e

$$\sum_e \int_{\Omega_0^e} \left(\mathbf{P}_M \cdot \boldsymbol{\nabla}_0 + \mathbf{B}_0 \right) \cdot \delta \mathbf{u}_M \, dV = 0$$



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$$\mathbf{N}_M = \mathbf{N}_M^-$$

$$\partial_I B_0 = \bigcup_e \partial \Omega_0^e$$

(Noels L. & Radovitzky R. IJNME 2006)

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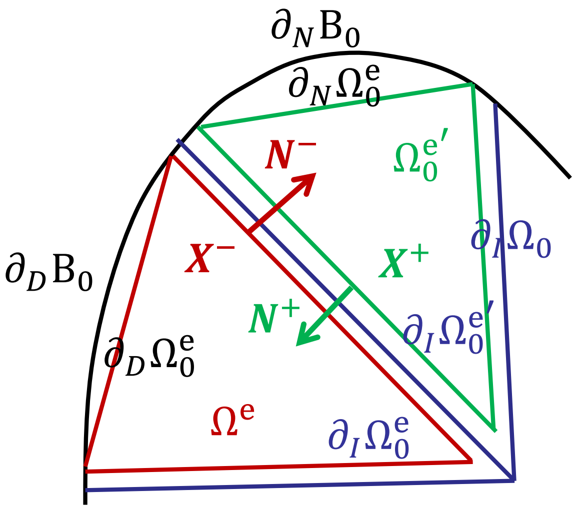
$$\sum_e \int_{\Omega_0^e} -\mathbf{P}_M : (\delta\mathbf{u}_M \otimes \boldsymbol{\nabla}_0) \, dV +$$
$$\sum_e \int_{\partial\Omega_0^e} \delta\mathbf{u}_M \cdot \mathbf{P}_M \cdot \mathbf{N}_M \, dA +$$
$$\sum_e \int_{\Omega_0^e} \mathbf{B}_0 \cdot \delta\mathbf{u}_M \, dV = 0$$



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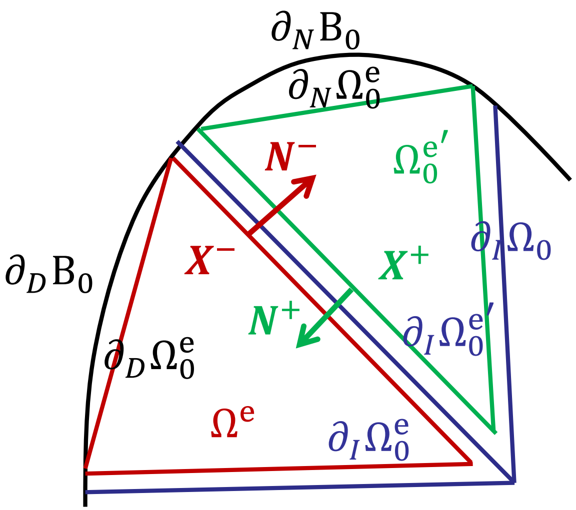

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$$\int_{B_0} \mathbf{P}_M : \left(\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0\right) \, dV +$$

$$\int_{\partial_I B_0} [\![\delta \mathbf{u}_M]\!] \cdot \langle \mathbf{P}_M \rangle \cdot \mathbf{N}_M \, dA =$$

$$\int_{B_0} \mathbf{B}_0 \cdot \delta \mathbf{u}_M \, dV + \int_{\partial_N B_0} \mathbf{T}_M^0 \cdot \delta \mathbf{u}_M \, dV$$

(Noels L. & Radovitzky R. IJNME 2006)

Discontinuous Galerkin formulation

- Displacement continuity is weakly enforced by DG interface terms

$$\int_{B_0} \mathbf{P}_M : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0)\ dV +$$
$$\int_{\partial_I B_0} [\![\delta \mathbf{u}_M]\!] \cdot \langle \mathbf{P}_M \rangle \cdot \mathbf{N}_M \, dA =$$
$$\int_{B_0} \mathbf{B}_0 \cdot \delta \mathbf{u}_M \, dV + \int_{\partial_N B_0} \mathbf{T}_M^0 \cdot \delta \mathbf{u}_M \, dV$$

Discontinuous Galerkin formulation

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β : stability parameter

h_s : characteristic mesh size

$\mathbf{L}^0_M$: tangent operator at zero deformation

$$\int_{B_0} \mathbf{P}_M : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0)\, dV + \int_{\partial_I B_0} [\![\delta \mathbf{u}_M]\!] \cdot \langle \mathbf{P}_M \rangle \cdot \mathbf{N}_M \, dA +$$

Compatibility term

$$\int_{\partial_I B_0} [\![\mathbf{u}_M]\!] \cdot \left\langle \mathbf{L}^0_M : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0) \right\rangle \cdot \mathbf{N}_M \, dA +$$

Stability term

$$\int_{\partial_I B_0} [\![\mathbf{u}_M]\!] \otimes \mathbf{N}_M : \left\langle \frac{\beta}{h_s} \mathbf{L}^0_M \right\rangle : [\![\delta \mathbf{u}_M]\!] \otimes \mathbf{N}_M \, dA =$$

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$$\int_{\partial_I B_0} [\![\mathbf{u}_M]\!] \otimes \mathbf{N}_M : \left\langle \frac{\beta}{h_s} \mathbf{L}^0_M \right\rangle : [\![\delta \mathbf{u}_M]\!] \otimes \mathbf{N}_M \, dA =$$

$$\int_{B_0} \mathbf{B}_0 \cdot \delta \mathbf{u}_M \, dV + \int_{\partial_N B_0} \mathbf{T}^0_M \cdot \delta \mathbf{u}_M \, dV$$

- Material constitutive relations must be provided

$$\mathbf{P}_M = \mathbf{P}_M \left(\mathbf{F}_M ; \mathbf{Q}_M \right)$$ →from microscopic analyses

Discontinuous Galerkin formulation

- Material constitutive relations are obtained from microscopic analyses
  - At integration points of both bulk and interface elements
  - First-order **FE^2** scheme

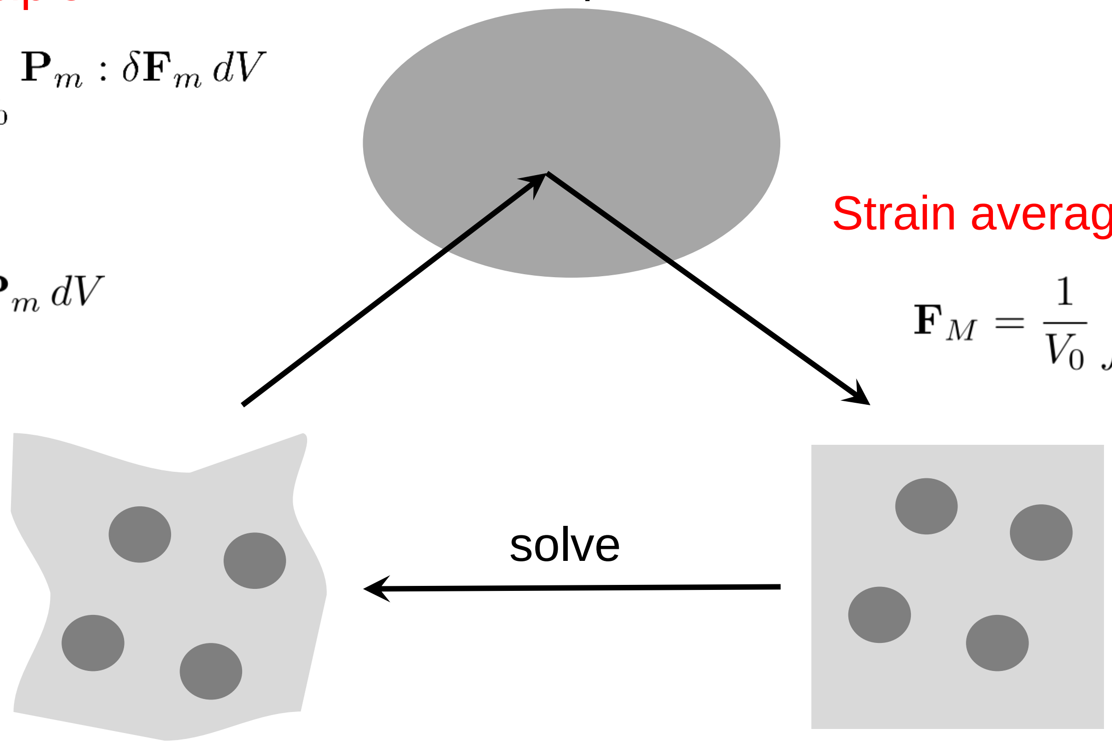
Hill-Mandel principle

$$\mathbf{P}_M : \delta\mathbf{F}_M = \frac{1}{V_0}\int_{V_0} \mathbf{P}_m : \delta\mathbf{F}_m \, dV$$

$$\mathbf{P}_M = \frac{1}{V_0}\int_{V_0} \mathbf{P}_m \, dV$$

$$\mathbf{L}_M = \frac{\partial \mathbf{P}_M}{\partial \mathbf{F}_M}$$

Macroscopic BVP



Strain averaging principle

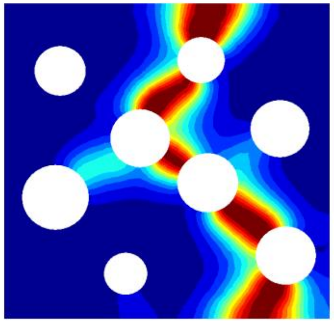
$$\mathbf{F}_M = \frac{1}{V_0}\int_{V_0} \mathbf{F}_m \, dV$$

Microscopic BVP

- Microscopic boundary condition: linear displacement, periodic, etc.

- Microscopic localization
  - Loss of ellipticity of the homogenized tangent operator

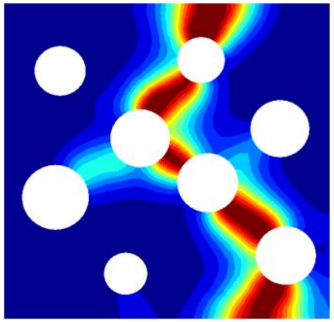
$$\min \operatorname{eig}\left(\mathbf{N}_M \cdot^2 \mathbf{L}_M \cdot \mathbf{N}_M\right) \leq 0$$



Local failure at the macroscopic scale

- Microscopic localization
  - Loss of ellipticity of the homogenized tangent operator

$$\min \operatorname{eig}\left(\mathbf{N}_M \cdot^2 \mathbf{L}_M \cdot \mathbf{N}_M\right) \leq 0$$



- Macroscale cohesive cracks need to be followed after the onset of microscopic strain localization

Discontinuous Galerkin formulation (DG) → Hybrid discontinuous Galerkin formulation / cohesive zone model (Hybrid DG/CZM)

Hybrid DG/CZM

- Discontinuity $\Gamma_0^D \subset \partial_I B_0$ is developed due to the microscopic localization
  - Cohesive cracks are meshed with interface elements

DG

$$\int_{B_0} \mathbf{P}_M : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0)\, dV + \int_{\partial_I B_0} [\![\delta \mathbf{u}_M]\!] \cdot \langle \mathbf{P}_M \rangle \cdot \mathbf{N}_M \, dA + \int_{\partial_I B_0} [\![\mathbf{u}_M]\!] \cdot \left\langle \mathbf{L}_M^0 : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0) \right\rangle \cdot \mathbf{N}_M \, dA + \int_{\partial_I B_0} [\![\mathbf{u}_M]\!] \otimes \mathbf{N}_M : \left\langle \frac{\beta}{h_s} \mathbf{L}_M^0 \right\rangle : [\![\delta \mathbf{u}_M]\!] \otimes \mathbf{N}_M \, dA = \int_{B_0} \mathbf{B}_0 \cdot \delta \mathbf{u}_M \, dV + \int_{\partial_N B_0} \mathbf{T}_M^0 \cdot \delta \mathbf{u}_M \, dV$$

Hybrid DG/CZM

$$\int_{B_0} \mathbf{P}_M : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0)\, dV + \int_{\partial_I B_0 \setminus \Gamma_0^D} [\![\delta \mathbf{u}_M]\!] \cdot \langle \mathbf{P}_M \rangle \cdot \mathbf{N}_M \, dA + \int_{\partial_I B_0 \setminus \Gamma_0^D} [\![\mathbf{u}_M]\!] \cdot \left\langle \mathbf{L}_M^0 : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0) \right\rangle \cdot \mathbf{N}_M \, dA + \int_{\partial_I B_0 \setminus \Gamma_0^D} [\![\mathbf{u}_M]\!] \otimes \mathbf{N}_M : \left\langle \frac{\beta}{h_s} \mathbf{L}_M^0 \right\rangle : [\![\delta \mathbf{u}_M]\!] \otimes \mathbf{N}_M \, dA + \int_{\Gamma_0^D} [\![\delta \mathbf{u}_M]\!] \cdot \mathbf{T}_M \, dA = \int_{B_0} \mathbf{B}_0 \cdot \delta \mathbf{u}_M \, dV + \int_{\partial_N B_0} \mathbf{T}_M^0 \cdot \delta \mathbf{u}_M \, dV$$

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Hybrid DG/CZM

$$\int_{B_0} \mathbf{P}_M : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0)\, dV + \int_{\partial_I B_0 \backslash \Gamma_0^D} [\![\delta \mathbf{u}_M]\!] \cdot \langle \mathbf{P}_M \rangle \cdot \mathbf{N}_M \, dA + \int_{\partial_I B_0 \backslash \Gamma_0^D} [\![\mathbf{u}_M]\!] \cdot \left\langle \mathbf{L}_M^0 : (\delta \mathbf{u}_M \otimes \boldsymbol{\nabla}_0) \right\rangle \cdot \mathbf{N}_M \, dA + \int_{\partial_I B_0 \backslash \Gamma_0^D} [\![\mathbf{u}_M]\!] \otimes \mathbf{N}_M : \left\langle \frac{\beta}{h_s} \mathbf{L}_M^0 \right\rangle : [\![\delta \mathbf{u}_M]\!] \otimes \mathbf{N}_M \, dA + \int_{\Gamma_0^D} [\![\delta \mathbf{u}_M]\!] \cdot \mathbf{T}_M \, dA = \int_{B_0} \mathbf{B}_0 \cdot \delta \mathbf{u}_M \, dV + \int_{\partial_N B_0} \mathbf{T}_M^0 \cdot \delta \mathbf{u}_M \, dV$$

- Cohesive constitutive relations on Γ_0^D must be provided

$$\mathbf{T}_M = \mathbf{T}_M \left(\mathbf{F}_M, [\![\mathbf{u}_M]\!] ; \mathbf{Q}_M \right)$$

→from microscopic analyses

- Homogenized cohesive law
  - Deformation of microscopic BVP is driven by an interface deformation gradient

$$\boldsymbol{\mathcal{F}}_M = \begin{cases} \mathbf{F}_M & \text{at onset of failure} \\ \boldsymbol{\mathcal{F}}_M\left(\mathbf{F}_M, [\![\mathbf{u}_M]\!]\right) & \text{after onset of failure} \end{cases}$$

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  - Cohesive traction is obtained from the first-order **FE²** scheme

Hill-Mandel principle

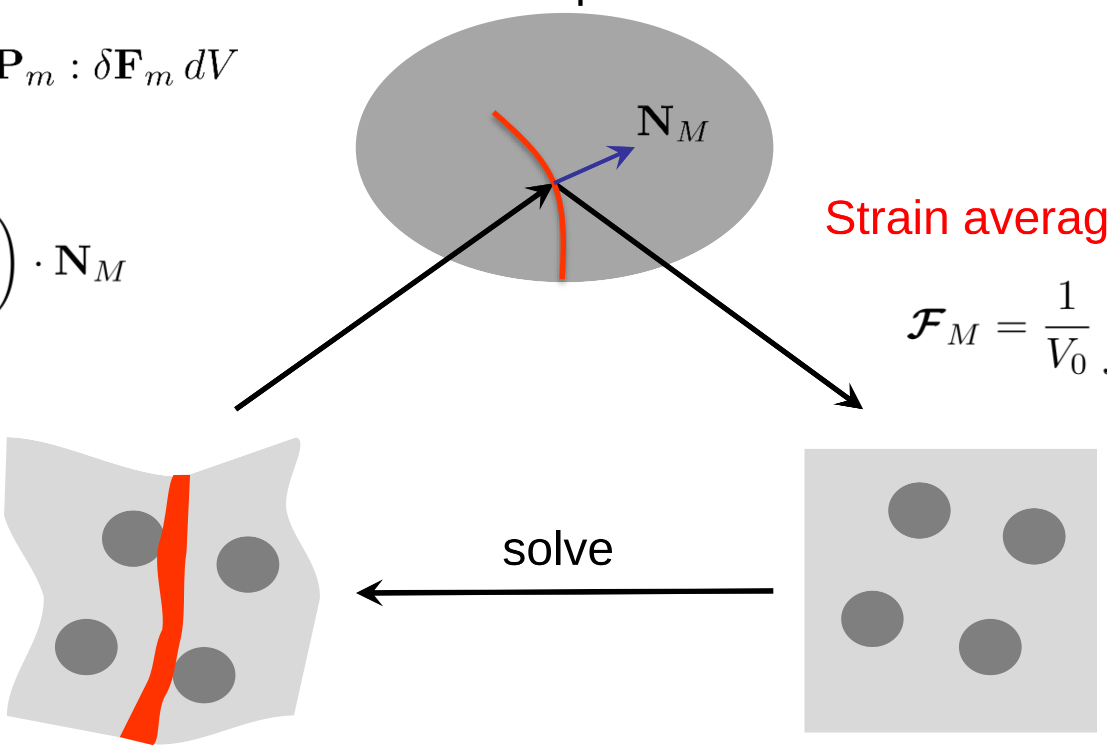
$$\mathbf{P}_M : \delta\boldsymbol{\mathcal{F}}_M = \frac{1}{V_0}\int_{V_0} \mathbf{P}_m : \delta\mathbf{F}_m \, dV$$

$$\mathbf{T}_M = \left(\frac{1}{V_0}\int_{V_0} \mathbf{P}_m \, dV\right)\cdot \mathbf{N}_M$$

$$\mathbf{K}_M = \frac{\partial \mathbf{T}_M}{\partial \boldsymbol{\mathcal{F}}_M} : \frac{\partial \boldsymbol{\mathcal{F}}_M}{\partial \mathbf{F}_M}$$

$$\mathbf{D}_M = \frac{\partial \mathbf{T}_M}{\partial \boldsymbol{\mathcal{F}}_M} : \frac{\partial \boldsymbol{\mathcal{F}}_M}{\partial [\![\mathbf{u}_M]\!]}$$

Macroscopic BVP



Strain averaging principle

$$\boldsymbol{\mathcal{F}}_M = \frac{1}{V_0}\int_{V_0} \mathbf{F}_m \, dV$$

- Homogenized cohesive law
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$$\boldsymbol{\mathcal{F}}_M = \begin{cases} \mathbf{F}_M & \text{at onset of failure} \\ \boldsymbol{\mathcal{F}}_M\left(\mathbf{F}_M, [\![\mathbf{u}_M]\!]\right) & \text{after onset of failure} \end{cases}$$

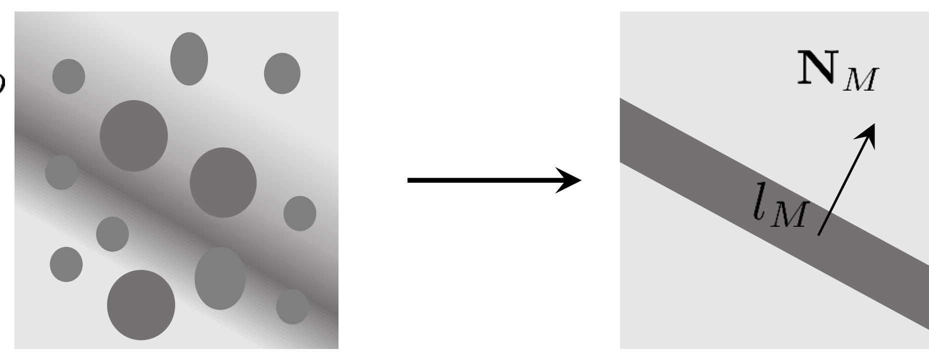
  - Active damage zone (Nguyen V.-P. et al. CMAME 2010)
    - Does not magnify with the microscopic volume element size
    - Has a constant width related to the nonlocal length scale

$$V_0^D = \{\mathbf{X} \in V_0 \mid \dot{D} > 0\} \qquad V_0^E = V_0 \backslash V_0^D \qquad \delta\mathbf{F}_M^{E,D} = \frac{1}{V_0^{E,D}} \int_{V_0^{E,D}} \delta\mathbf{F}_m \, dV$$

  - Cohesive jump is homogenized from the microscopic localization strain inside the active damage zone

$$\delta\mathbf{F}_M^D = \frac{1}{l_M} \delta\left[\!\left[\mathbf{u}_M\right]\!\right] \otimes \mathbf{N}_M$$

V_0^D



l_M: average band width

Hybrid DG/CZM

- Homogenized cohesive law
  - Deformation of microscopic BVP is driven by an interface deformation gradient

$$\boldsymbol{\mathcal{F}}_M = \begin{cases} \mathbf{F}_M & \text{at onset of failure} \\ \boldsymbol{\mathcal{F}}_M\left(\mathbf{F}_M, [\![\mathbf{u}_M]\!]\right) & \text{after onset of failure} \end{cases}$$

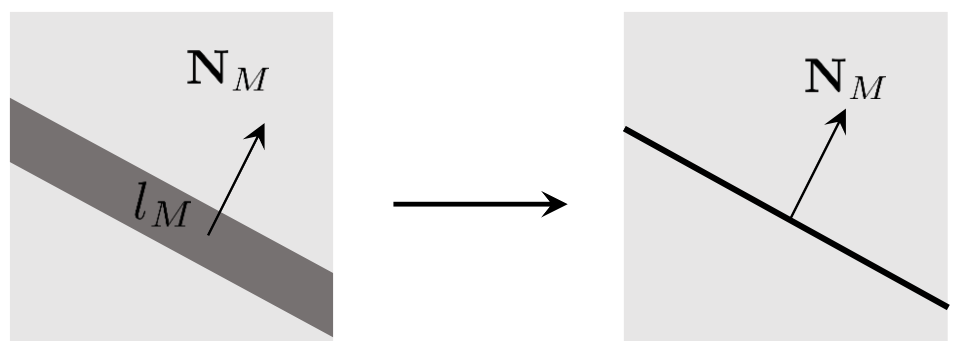
  - Strain averaging principle

$$\begin{aligned} \delta\boldsymbol{\mathcal{F}}_M &= \frac{1}{V_0}\int_{V_0} \delta\mathbf{F}_m \, dV \\ &= (1-\beta)\delta\mathbf{F}_M^E + \beta\delta\mathbf{F}_M^D \end{aligned}$$

$$\begin{cases} (1-\beta)\,\delta\mathbf{F}_M^E & = \delta\mathbf{F}_M \\ \delta\mathbf{F}_M^D & = \frac{1}{l_M}\delta\,[\![\mathbf{u}_M]\!] \otimes \mathbf{N}_M \end{cases}$$

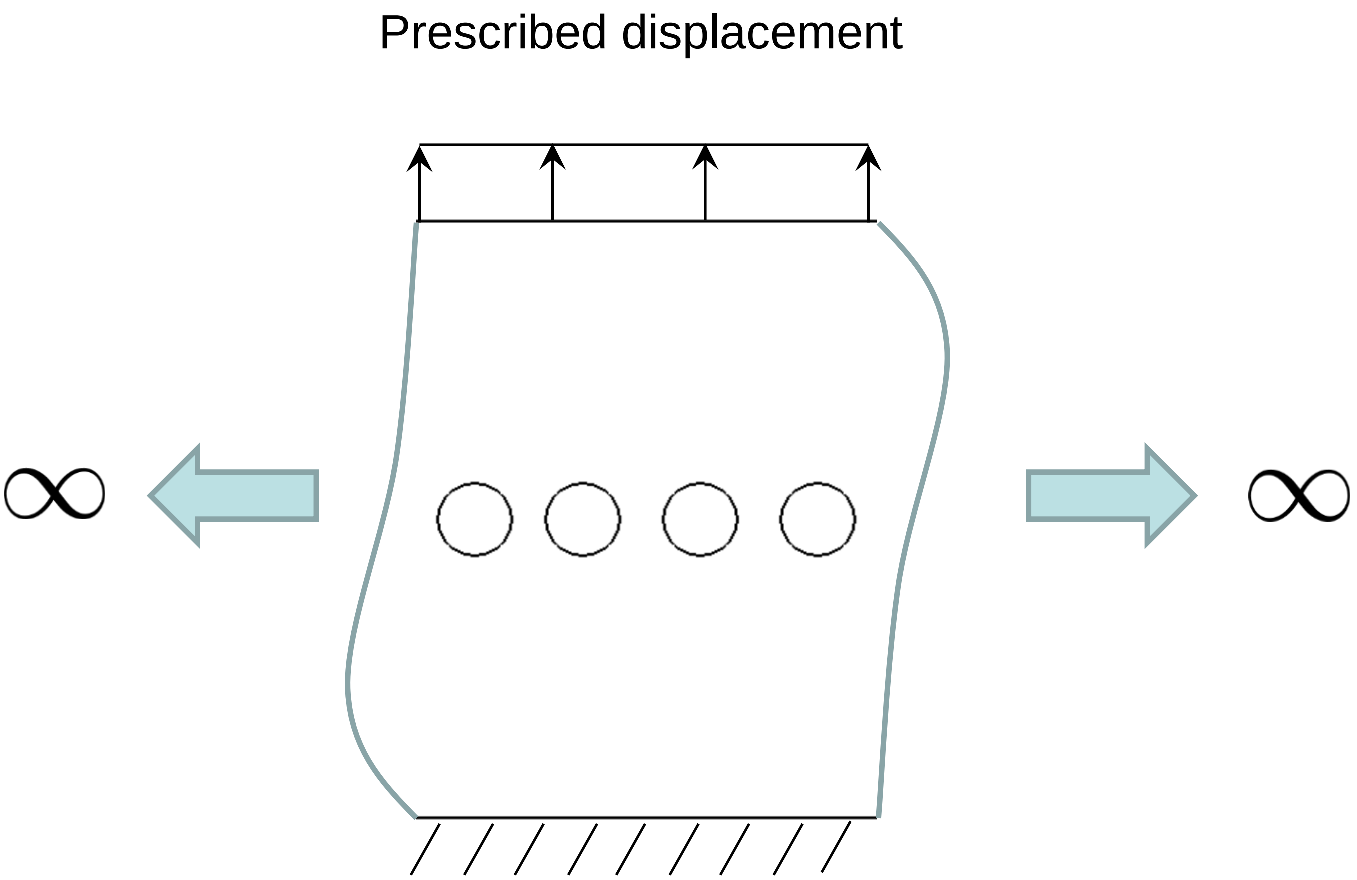
$$\delta\boldsymbol{\mathcal{F}}_M = \delta\mathbf{F}_M + \frac{\beta}{l_M}\delta\,[\![\mathbf{u}_M]\!] \otimes \mathbf{N}_M$$

$$\beta = \frac{V_0^D}{V_0}$$



Macro-crack

- Uniaxial test
  - Non-local elastoplastic-damage material law



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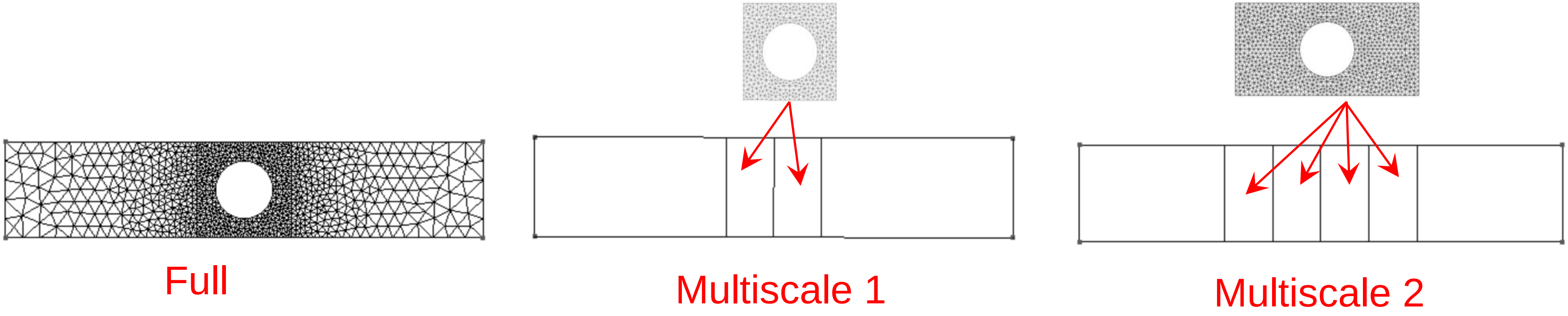
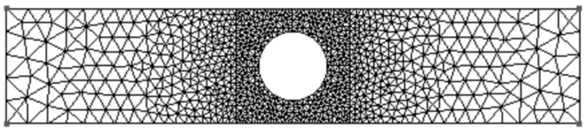
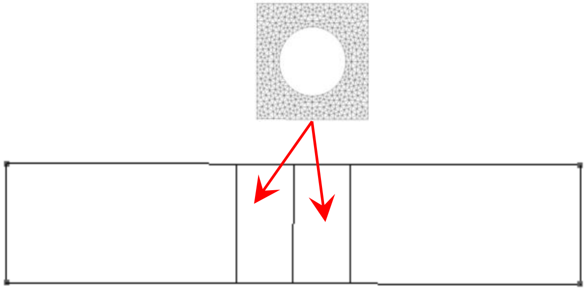


Numerical examples

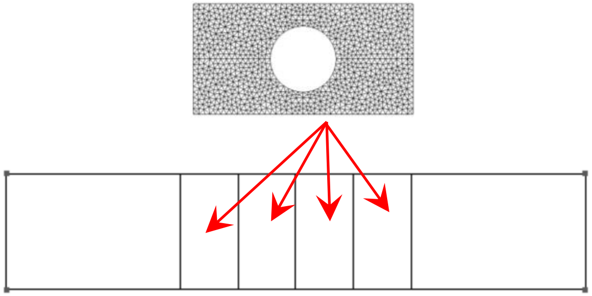
- Uniaxial test
  - Non-local elastoplastic-damage material law



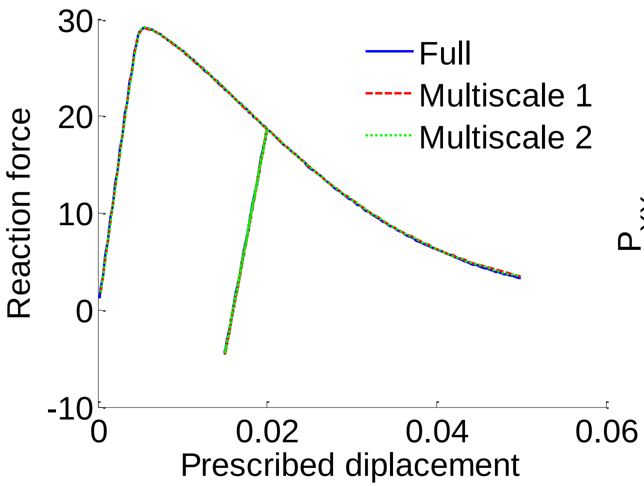
Full



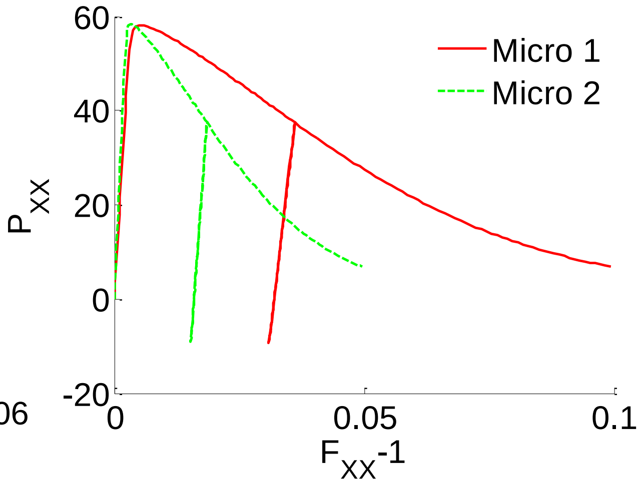
Multiscale 1



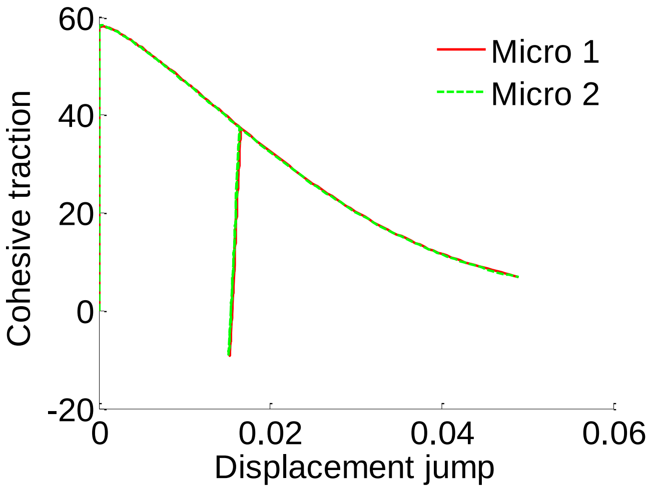
Multiscale 2



Macroscopic response

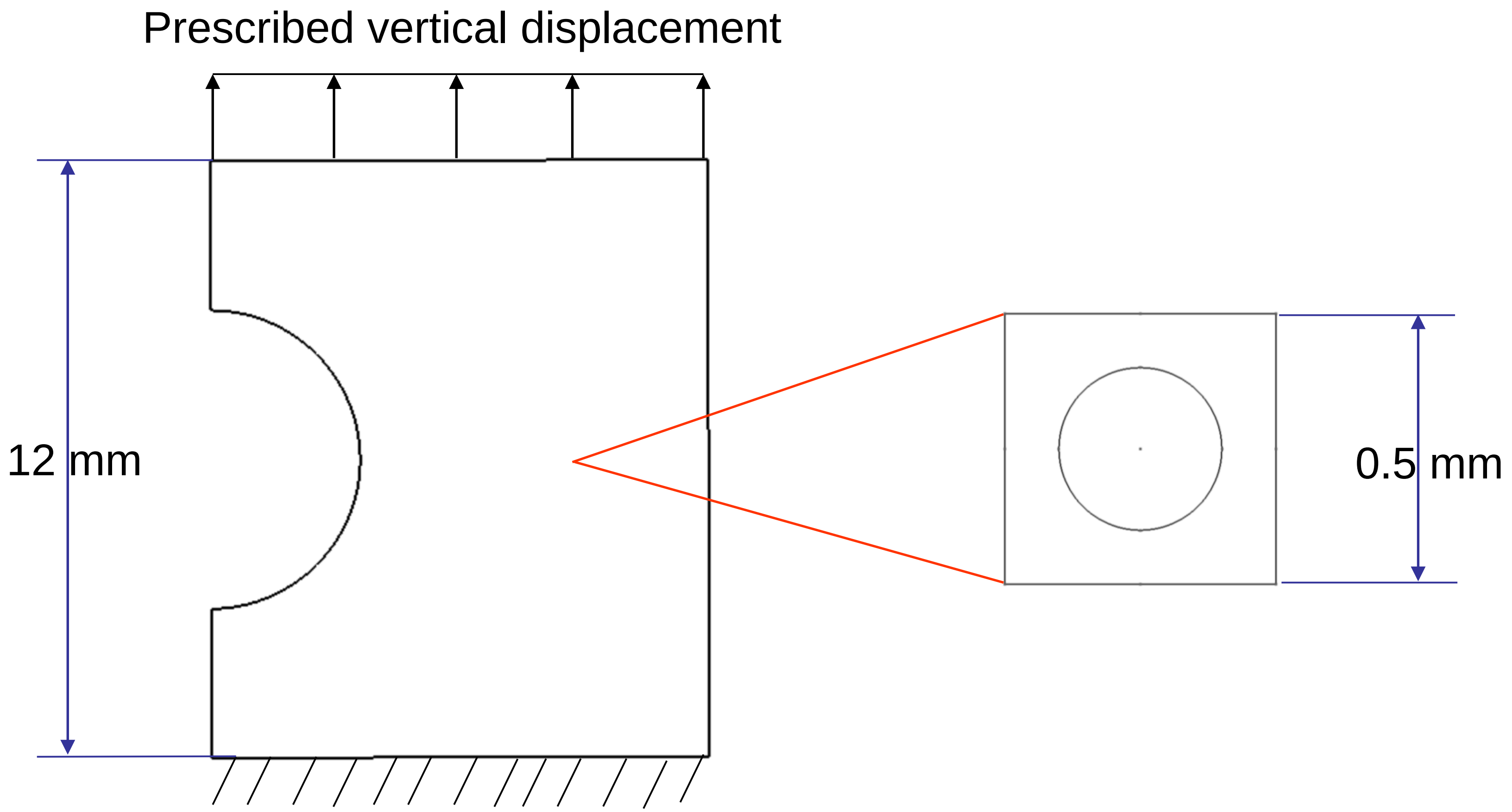


Homogenized stress-strain response



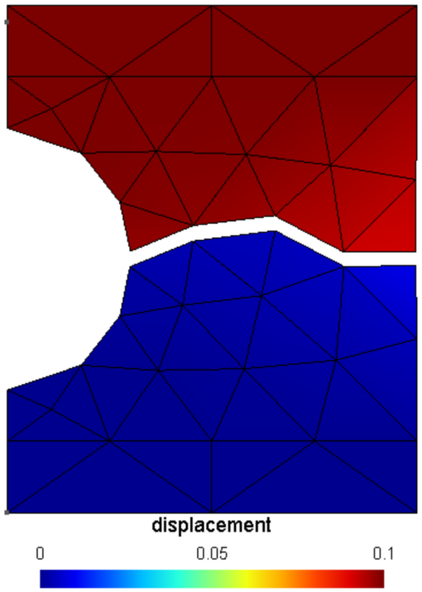
Homogenized cohesive response

- Notched sample
  - Non-local elastoplastic-damage material law

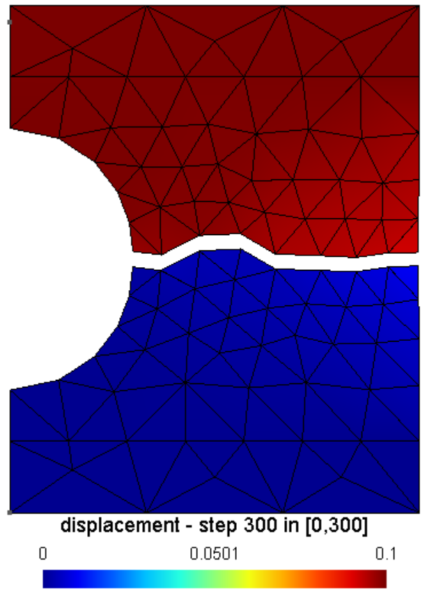


Numerical examples

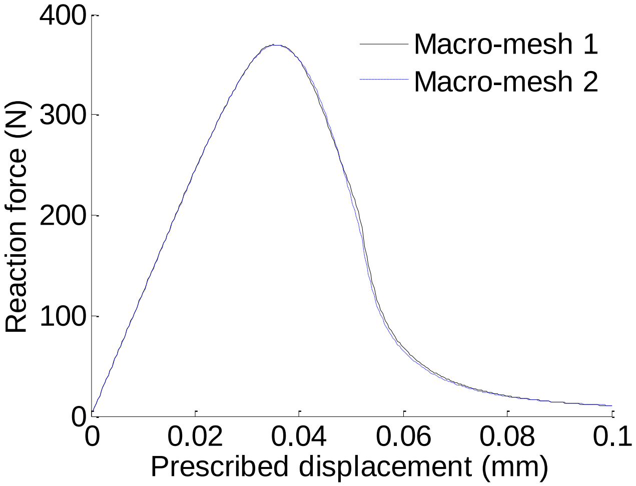
- Notched sample
  - Non-local elastoplastic-damage material law



Macro-mesh 1



Macro-mesh 2



Conclusions

- This proposed FE^2 scheme is based on the DG/CZM framework
  - Extrinsic cohesive zone model
  - Cohesive normal is known
- Both bulk and interface constitutive relations are obtained from microscopic analyses at finite strains
- The triaxiality effect during the failure process is automatically accounted for since both the macroscopic deformation gradient and macroscopic displacement jump are used to formulation the microscopic BVP

Thank you for your attention !