A multiscale computational scheme based on a hybrid discontinuous Galerkin/cohesive zone model for damage and failure of microstructured materials

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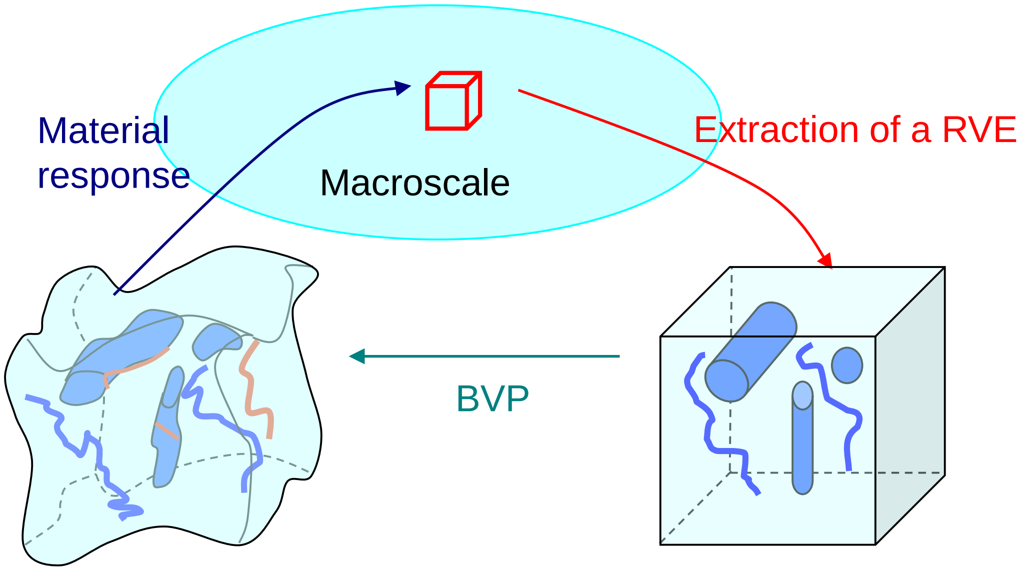
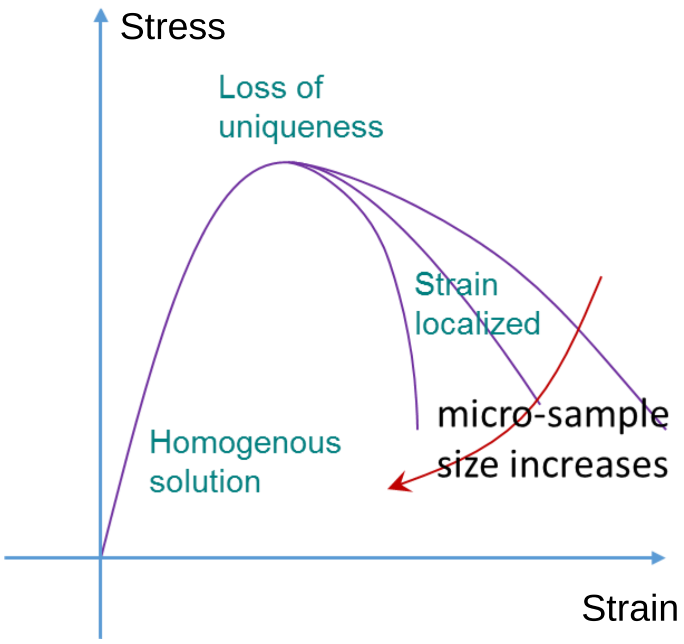
- Computational homogenization (so-called FE^2) for micro-structured materials
  - Two boundary value problems (BVP) are concurrently solved
    - Macroscale BVP
    - Microscale BVP
      - Representative Volume Elements (RVE) are extracted from material microstructure
      - An appropriate boundary condition
  - Separation of length scales $L_{\text{macro}} \gg L_{\text{RVE}} \gg L_{\text{micro}}$



Conventional FE^2 scheme

- 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



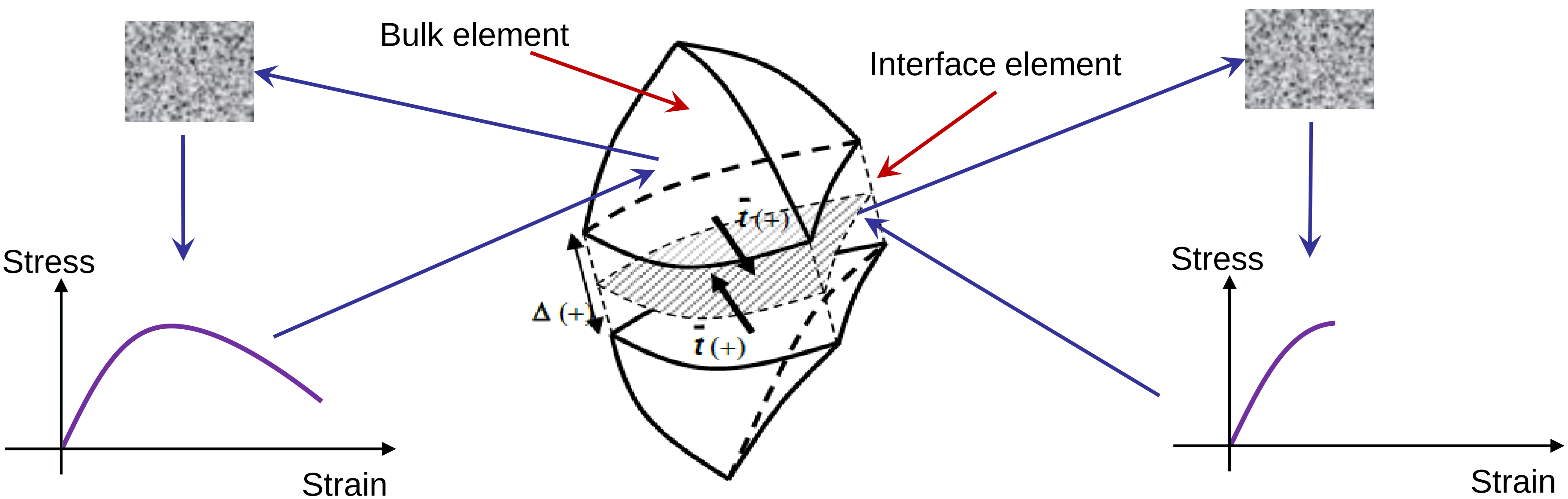
→Solution: FE^2 with enhanced discontinuity (continuous-discontinuous FE^2)

  - Macroscale cohesive crack is inserted after onset of microscopic strain localization
  - Cohesive law is extracted from microscale BVP

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

Computational strategy

- FE^2 with enhanced discontinuity based on Discontinuous-Galerkin/ Extrinsic cohesive zone model (DG/ECZM) formulation
  - Failure is detected at interface elements
  - Prior to the microscopic strain localization:
    - FE^2 based on DG formulation (Nguyen V.-D. et al. CMAME 2013)



Homogenized bulk law

At the macroscale

Homogenized interface law

Computational strategy

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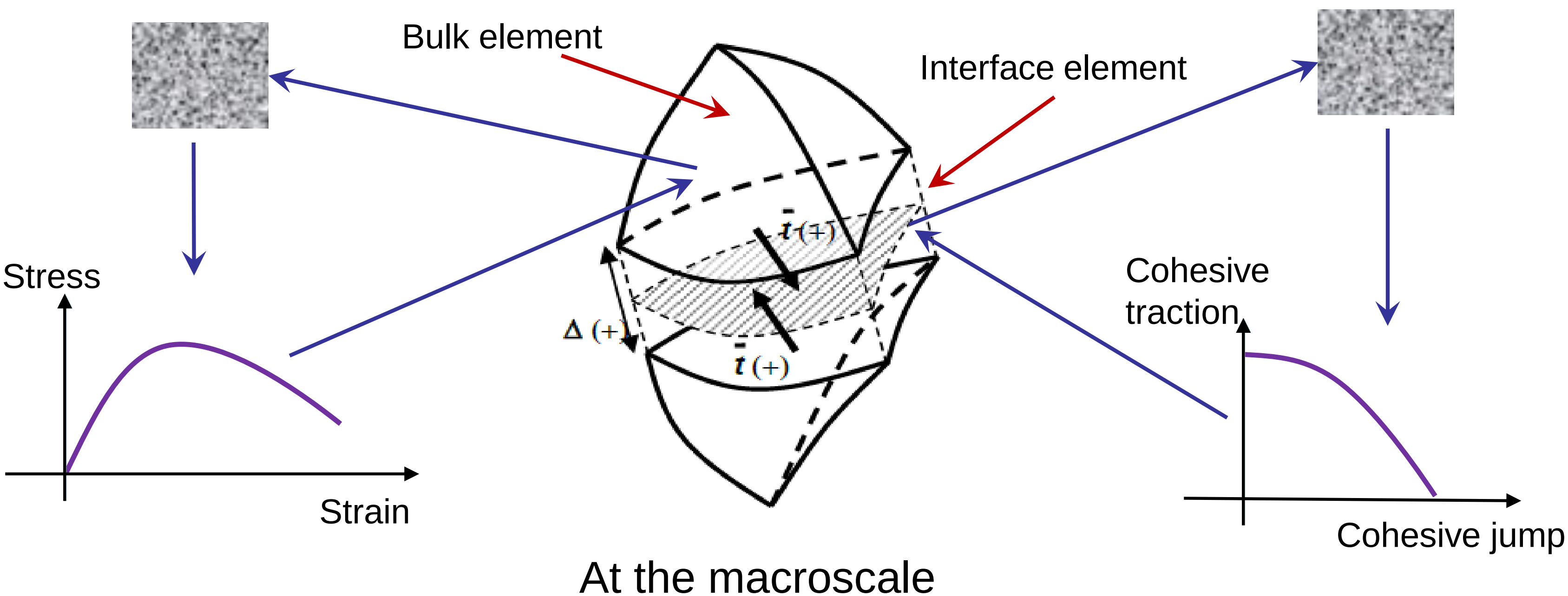
  - Prior to the microscopic strain localization:
    - FE^2 based on DG formulation (Nguyen V.-D. et al. CMAME 2013)
  - After the onset of microscopic strain localization:
    - FE^2 based on DG/ECZM formulation
      - Cohesive crack is inserted after onset of microscopic localization
      - Extrinsic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



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  - After the onset of microscopic strain localization:
    - FE^2 based on DG/ECZM formulation
      - Cohesive crack is inserted after onset of microscopic localization
      - Extrinsic cohesive law is extracted from microscopic damage
  - Advantages
    - Same discontinuous polynomial approximations are considered for the test and trial functions
    - Mesh topology does not change during simulations
    - Microscopic BVPs at bulk and interface integration points are inserted from the beginning of simulations
    - Cohesive normal is known

Content

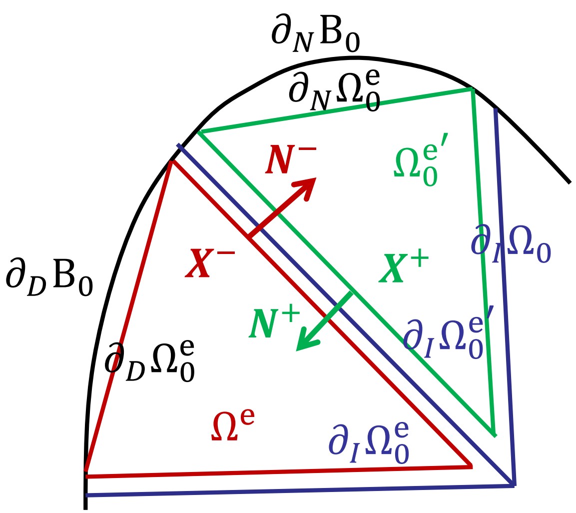
- Macroscopic hybrid DG/CZM formulation
- Microscopic implicit non-local damage formulation
- Extraction of the cohesive law from microscopic localization
- Homogenization-based multi-scale analysis
- Conclusions

Macroscopic hybrid DG/CZM formulation

- Strong form formulated in terms of the first Piola Kirchhoff stress

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

- Weak form obtained by applying integration by parts on each element Ω_0^e



$$\begin{cases} \text{Jump operator } [\![\bullet]\!] = \bullet^+ - \bullet^- \\ \text{Mean operator } \langle\bullet\rangle = \frac{1}{2}\left(\bullet^+ + \bullet^-\right) \end{cases}$$

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

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

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

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

$$\mathbf{T}_M = \langle \mathbf{P}_M \rangle \cdot \mathbf{N}_M$$

(Noels L. & Radovitzky R. IJNME 2006)

Macroscopic hybrid DG/CZM formulation

- Prior to the onset of microscopic localization
  - Displacement continuity enforced by DG interface terms

(Noels L. & Radovitzky R. IJNME 2006)

Bulk term → $$\int_{B_0} \mathbf{P}_M : \delta\mathbf{u}_M \otimes \boldsymbol{\nabla}_0 \, dV +$$

Interface consistency term → $$\int_{\partial_I B_0} \mathbf{T}_M \cdot [\![\delta\mathbf{u}_M]\!] \, dA +$$

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

Interface stability term → $$\int_{\partial_I B_0} [\![\mathbf{u}_M]\!] \cdot \mathbf{S}^h \cdot [\![\delta\mathbf{u}_M]\!] \, dA$$

External force terms → $$= \int_{\partial_N B_0} \mathbf{T}^0_M \cdot \delta\mathbf{u}_M \, dA + \int_{B_0} \mathbf{B}_0 \cdot \delta\mathbf{u}_M \, dV$$

Macroscopic hybrid DG/CZM formulation

- After the onset of microscopic localization
  - The equality between the homogenized cohesive jump and the macroscopic displacement jump is enforced by DG interface terms

(Truster T.J. & Masud A. Comp. Mech. 2013, Hansbo P. & Salomonsson K. FEAD 2016)

Bulk term → $$\int_{B_0} \mathbf{P}_M : \delta\mathbf{u}_M \otimes \boldsymbol{\nabla}_0 \, dV +$$

Interface consistency term → $$\int_{\partial_I B_0} \mathbf{T}_M \cdot [\![\delta\mathbf{u}_M]\!] \, dA +$$

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

Interface stability term → $$\int_{\partial_I B_0} \left([\![\mathbf{u}_M]\!] - \boldsymbol{\Delta}_M\right) \cdot \mathbf{S}^{h*} \cdot \left[[\![\delta\mathbf{u}_M]\!] - \left\langle \mathbf{S}^0_F : (\delta\mathbf{u}_M \otimes \boldsymbol{\nabla}_0)\right\rangle\right] dA$$

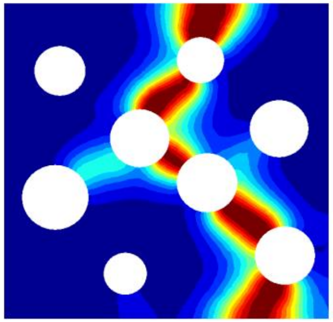
External force terms → $$= \int_{\partial_N B_0} \mathbf{T}^0_M \cdot \delta\mathbf{u}_M \, dA + \int_{B_0} \mathbf{B}_0 \cdot \delta\mathbf{u}_M \, dV$$

  - Homogenized extrinsic cohesive law from microscopic BVP
    - Cohesive jump: $\boldsymbol{\Delta}_M = \boldsymbol{\Delta}_M \left(\langle \mathbf{F}_M \rangle, [\![\mathbf{u}_M]\!]\right)$
    - Cohesive traction: $\mathbf{T}_M = \mathbf{T}_M \left(\langle \mathbf{F}_M \rangle, [\![\mathbf{u}_M]\!]\right)$

Microscopic implicit non-local damage formulation

- Strong form
$$\begin{cases}\mathbf{P}_m \cdot \boldsymbol{\nabla}_0 = \mathbf{0} \\ \bar{\varphi} - c\Delta\bar{\varphi} = \varphi\end{cases} \quad \text{on } V_0$$
  - Microscopic constitutive laws
$$\begin{cases}\mathbf{P}_m &= (1-D)\hat{\mathbf{P}}_m \\ D &= D\left(\bar{\varphi}, \mathbf{F}_m, \mathbf{Q}\right) \\ \hat{\mathbf{P}}_m &= \hat{\mathbf{P}}_m\left(\mathbf{F}_m, \mathbf{Q}\right)\end{cases}$$

- Active damage zone
  - Does not magnify with the microscopic volume element size
  - Has a constant width related to the parameter c



$$V_0^D = \{\mathbf{X} \in V_0 \mid \dot{\gamma} > 0 \text{ and } \dot{D} > 0\} \qquad V_0^E = V_0 \backslash V_0^D$$

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

(Nguyen V.-P. et al. CMAME 2010)

Microscopic implicit non-local damage formulation

- Macro-micro transition

$$\boldsymbol{\mathcal{F}}_M = \langle \mathbf{F}_M \rangle + \beta_M [\![\mathbf{u}_M]\!] \otimes \mathbf{N}_M = \frac{1}{V_0}\int_{V_0} \mathbf{F}_m \, dV$$

(Coenen E. et al. JMPS 2012)

  - $\mathbf{N}_M$ is known as the normal of interface elements

- Hill- Mandel principle

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

- Micro-macro transition

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

  - Cohesive traction $\mathbf{T}_M = \mathbf{P}_M \cdot \mathbf{N}_M$
  - Onset of microscopic localization $\min \operatorname{eig}\left(\mathbf{N}_M \cdot^2 \mathbf{L}_M \cdot \mathbf{N}_M\right) \leq 0$
  - Prior to the onset of microscopic localization $\boldsymbol{\Delta}_M = 0$
  - After the onset of microscopic localization → extract cohesive law

Extraction cohesive law from microscopic localization

- Homogenized cohesive jump
  - Variational form

$$\delta \mathbf{\Delta}_M = l \delta \mathbf{F}_M^D \cdot \mathbf{N}_M$$

  - Integration form

$$\Delta_M = \int_{\mathbf{F}_M^{D0}}^{\mathbf{F}_M^D} l \delta \mathbf{F}_M^D \cdot \mathbf{N}_M$$

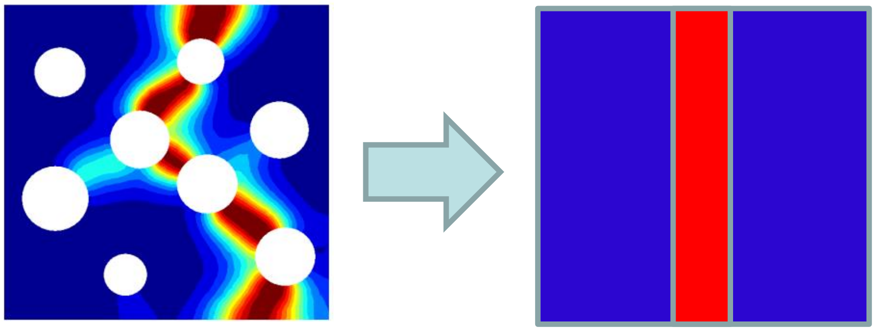
Value at the failure onset

(Nguyen V.-P. et al. CMAME 2010)

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

Average band width

$$l \approx \beta^D L_0$$



$$V_0^D = \{\mathbf{X} \in V_0 \mid \dot{\gamma} > 0 \text{ and } \dot{D} > 0\} \qquad V_0^E = V_0 \backslash V_0^D$$

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

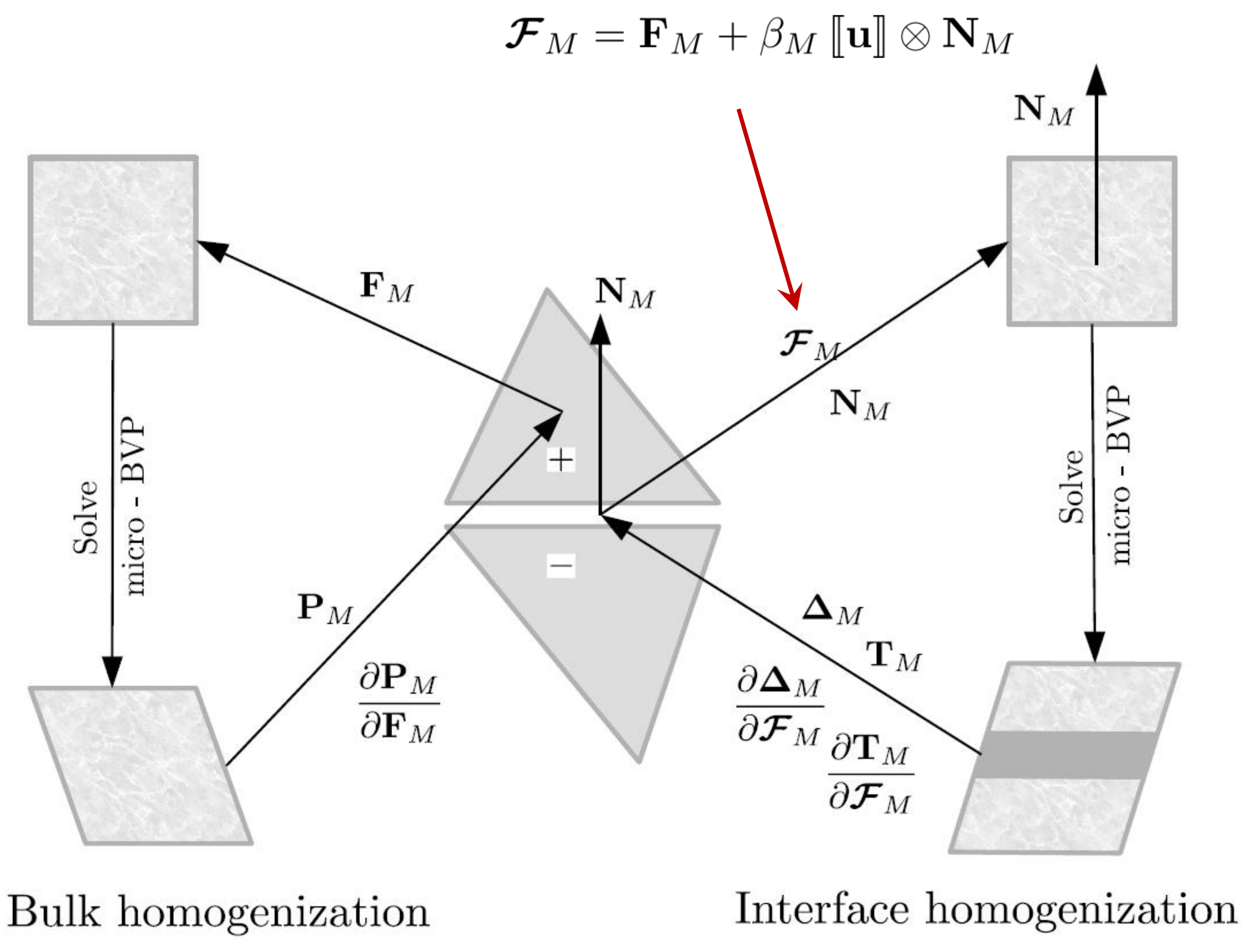
- Macro-micro transition

$$\begin{aligned} \langle \delta \mathbf{F}_M \rangle + \beta_M [\![\delta \mathbf{u}_M]\!] \otimes \mathbf{N}_M &= \left(1 - \beta^D\right) \delta \mathbf{F}_M^E + \beta^D \delta \mathbf{F}_M^D \\ &= \left(1 - \beta^D\right) \delta \mathbf{F}_M^E + \frac{\beta^D}{l} \delta \mathbf{\Delta}_M \otimes \mathbf{N}_M \end{aligned}$$

$$\rightarrow \begin{cases} \langle \delta \mathbf{F}_M \rangle = \left(1 - \beta^D\right) \delta \mathbf{F}_M^E \\ \beta_M = \frac{\beta^D}{l} \approx \frac{1}{L_0} \end{cases}$$

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

- Two-scale concurrent scheme

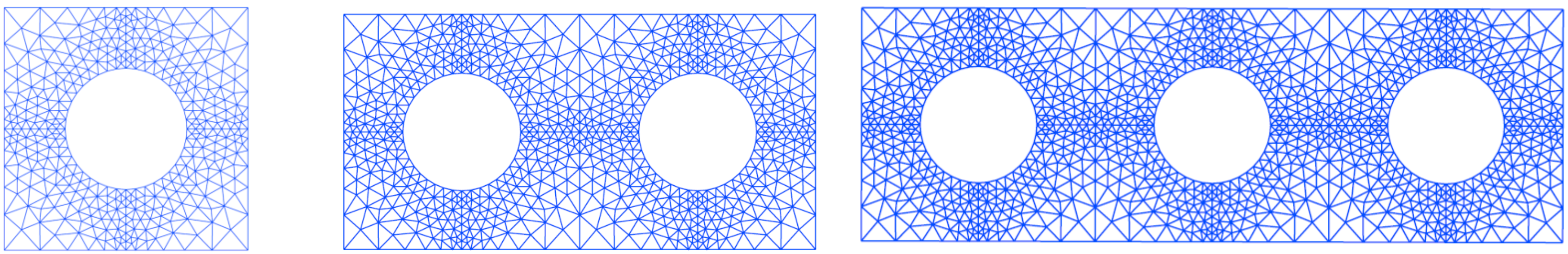


- First result: homogenized extrinsic cohesive law
  - Pure opening mode

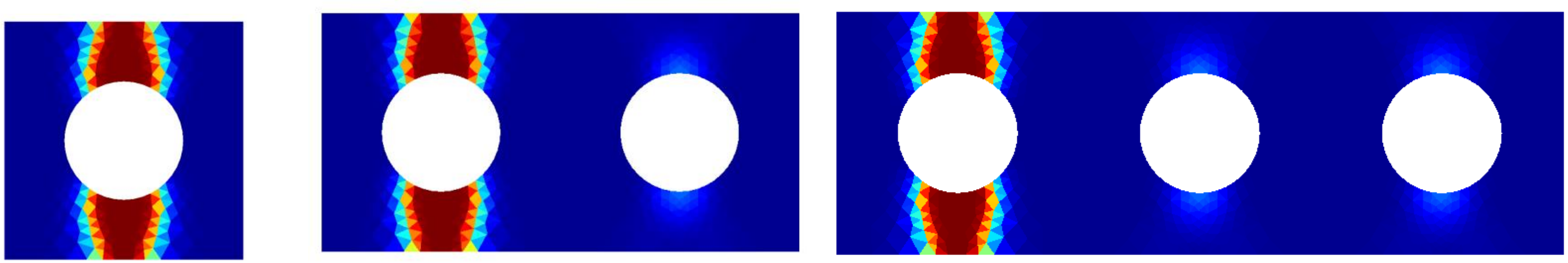
$$\mathcal{F}_M = \begin{bmatrix} 1+\lambda & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

  - RVE geometries

RVE 1 | RVE 2 | RVE 3



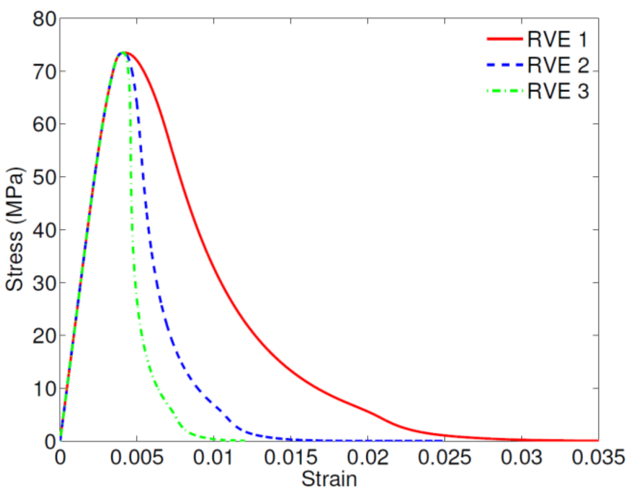
  - Damage pattern



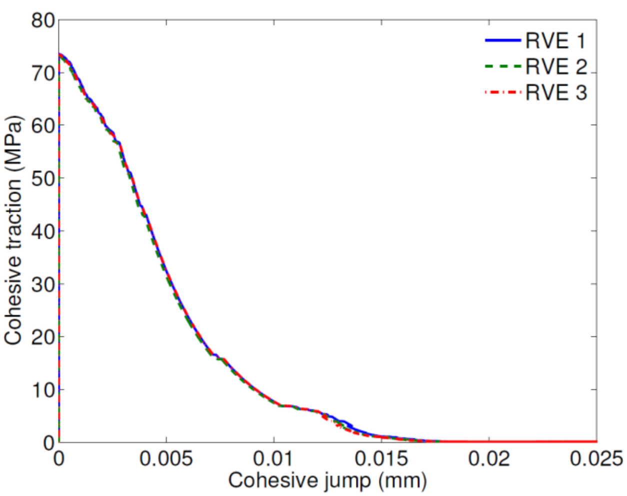
- First result: homogenized extrinsic cohesive law
  - Pure opening mode

$$\mathcal{F}_M = \begin{bmatrix} 1+\lambda & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

  - Objective homogenized extrinsic cohesive law



Stress-strain response

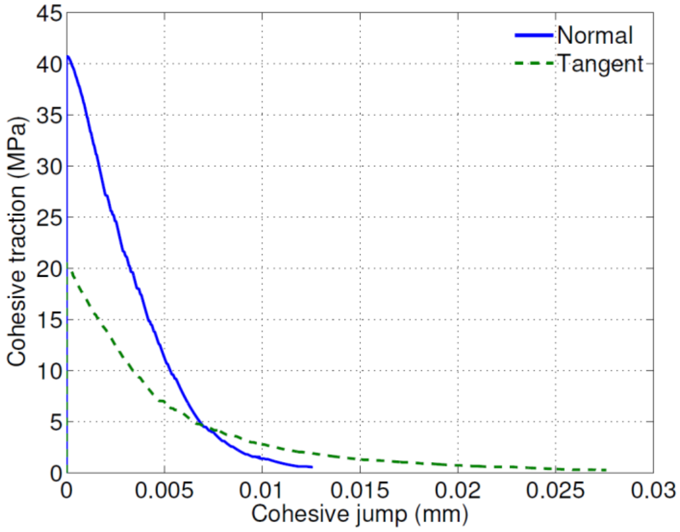


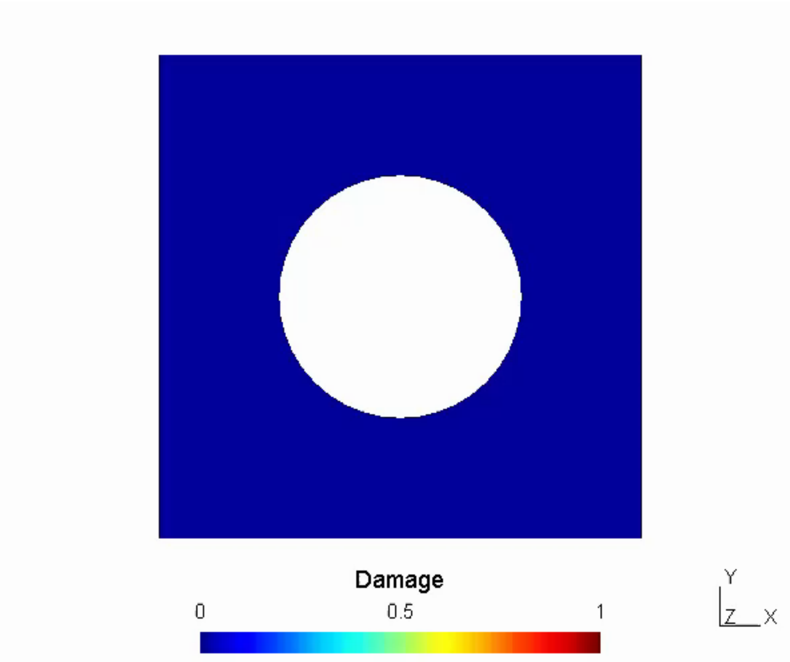
Cohesive response

- First result: homogenized extrinsic cohesive law
  - Mixed mode

$$\boldsymbol{\mathcal{F}}_M = \begin{bmatrix} 1+\lambda & 0 & 0 \\ 2\lambda & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

  - Homogenized extrinsic cohesive law





Conclusions

- This proposed FE^2 scheme is based on the DG/ECZM framework
  - Extrinsic cohesive law
  - Cohesive normal is known
- Both bulk and interface constitutive relations are obtained from microscopic analyses at finite strains
- The equality between the cohesive jump and the displacement jump is ensured by having recourse to the DG formulation
- 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
- Future works
  - Two-scale simulations
  - Application to composites by incorporate matrix damage with matrix-fiber decohesion
  - Validation by experiments

Thank you for your attention !