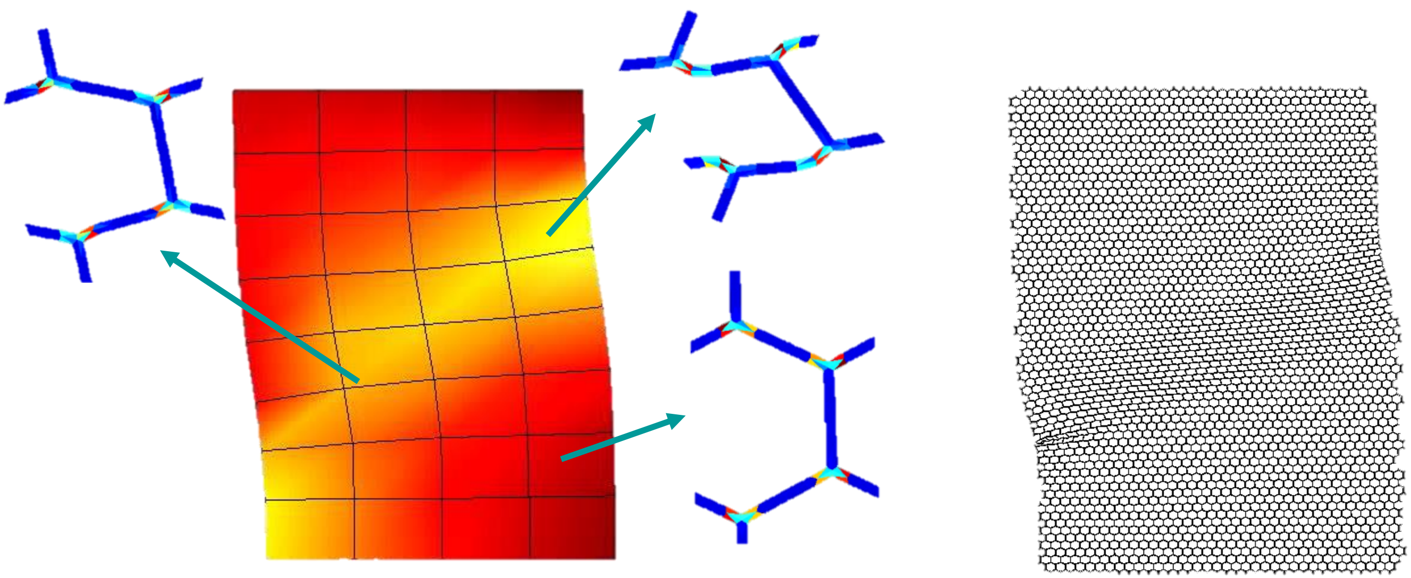
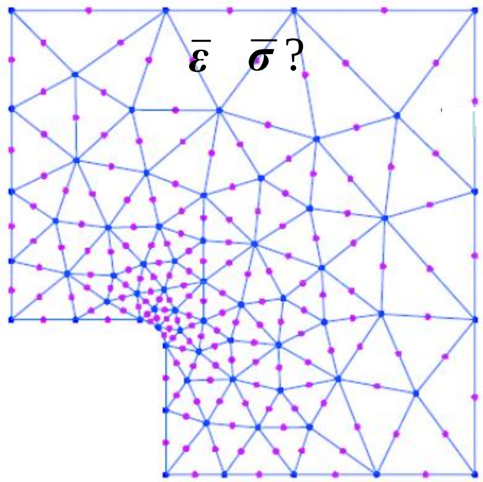
# Computational homogenization of cellular materials with propagation of instabilities through the scales

V.-D. Nguyen, F. Wan, J.-M. Thomassin, L. Noels



Les recherches ont été financées grâce à la subvention “Actions de recherche concertées ARC 09/14-02 BRIDGING- From imaging to geometrical modelling of complex micro structured materials: Bridging computational engineering and material science

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



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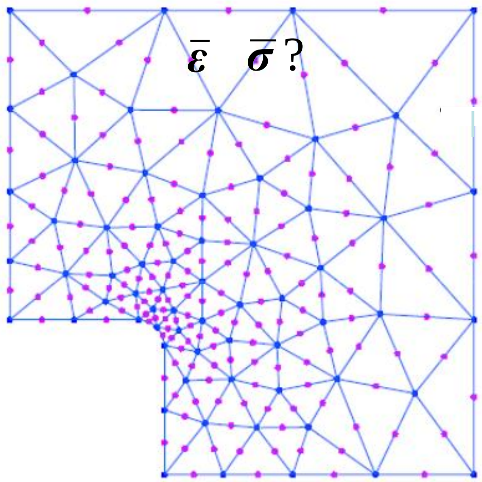
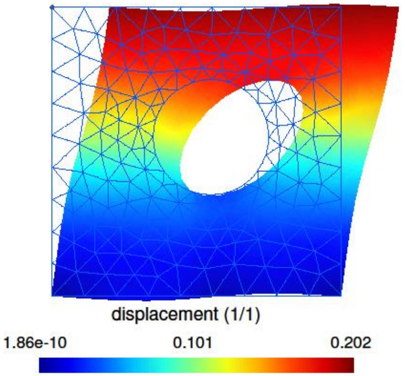
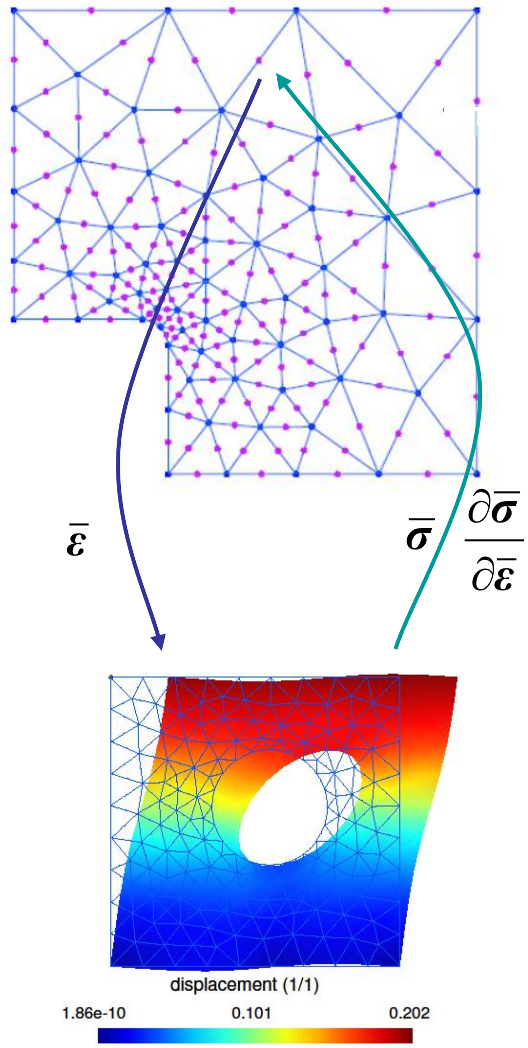



  - Micro-scale
    - Usual 3D finite elements
    - Periodic boundary conditions



# Multi-scale modelling: How?

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



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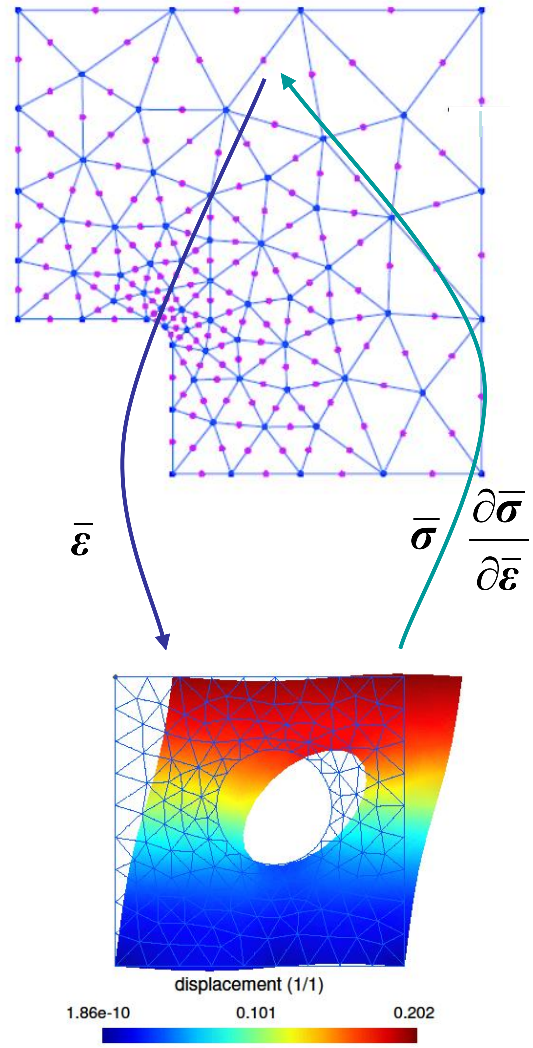
  - Micro-scale
    - Usual 3D finite elements
    - Periodic boundary conditions
  - Advantages
    - Accuracy
    - Generality
  - Drawback
    - Computational time

**Assumptions:**

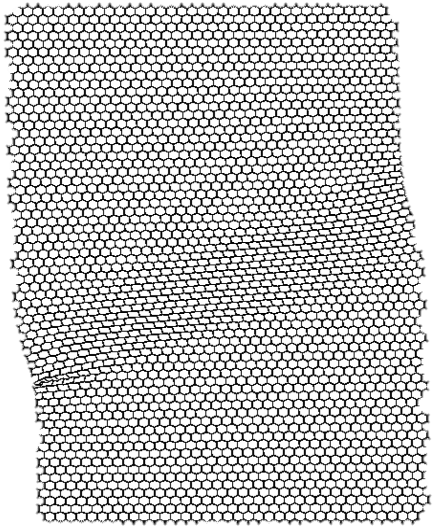
$L_{macro} >> L_{RVE} >> L_{micro}$




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

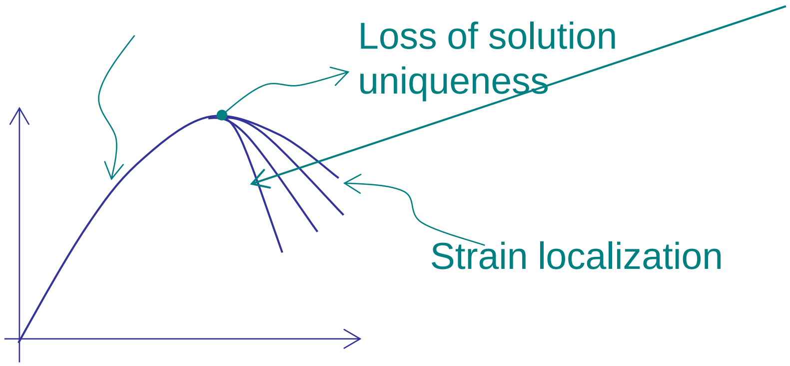
# Multi-scale simulations with strain softening

- Propagation of instabilities in honeycomb structures
  - Due to micro-buckling
  - Localization bands

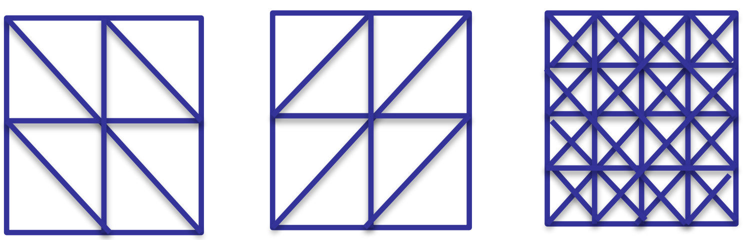


- Finite element solutions for strain softening problems suffer from:
  - Loss of solution uniqueness and strain localization
  - Mesh dependence

Homogeneous unique solution




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

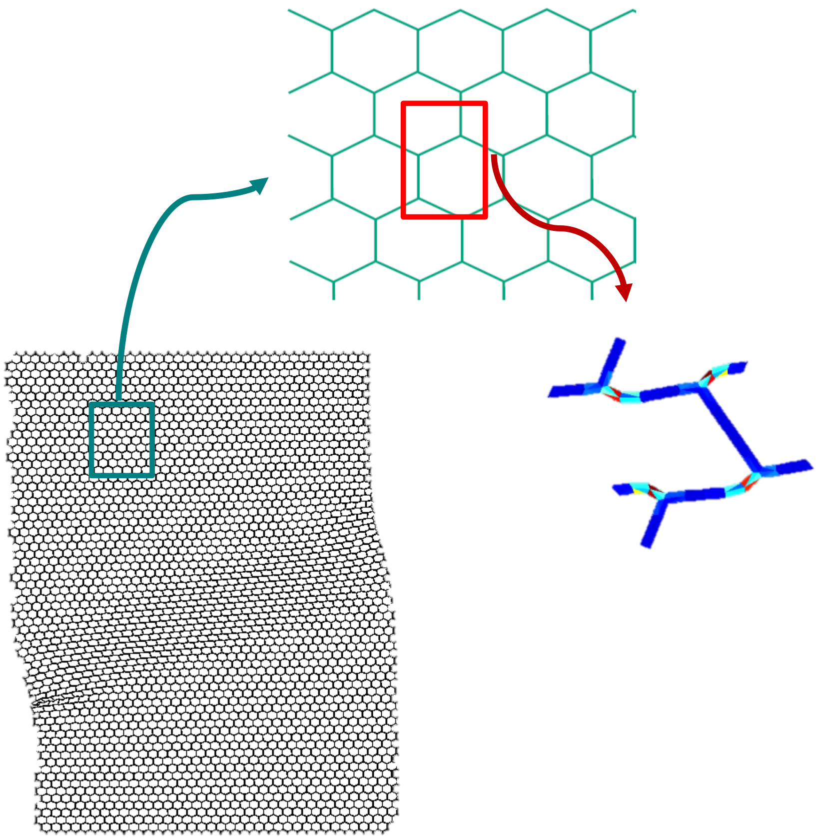


The numerical results change without convergence

# Computational homogenization for foamed materials

- Challenges
  - Micro-structure
    - Not perfect with non periodic mesh

⇨ How to constrain the periodic boundary conditions?



# Computational homogenization for foamed materials

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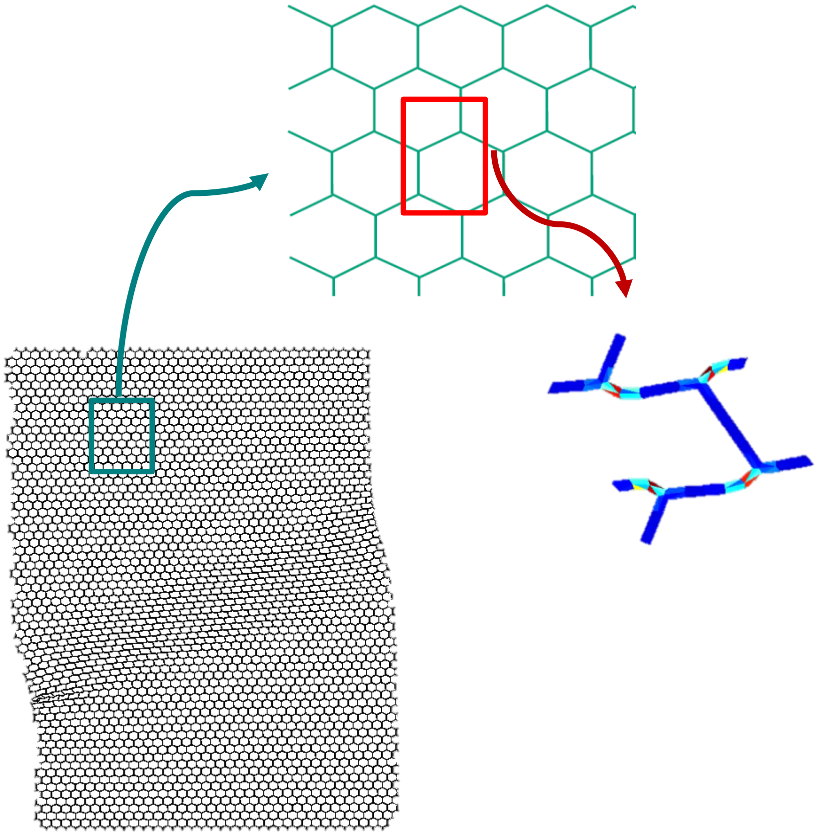
    - Thin components
    - Experiences micro-buckling

      ⇨ How to capture the instability?



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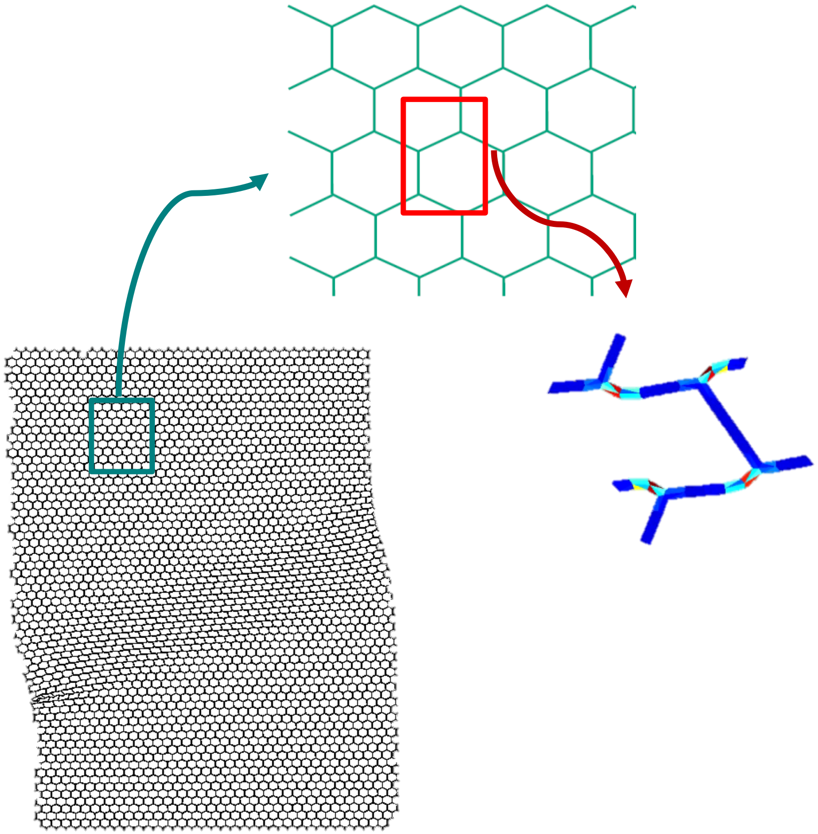
  - Transition
    - Homogenized tangent not always elliptic
    - Localization bands

      ⇨ How can we recover the solution unicity at the macro-scale?



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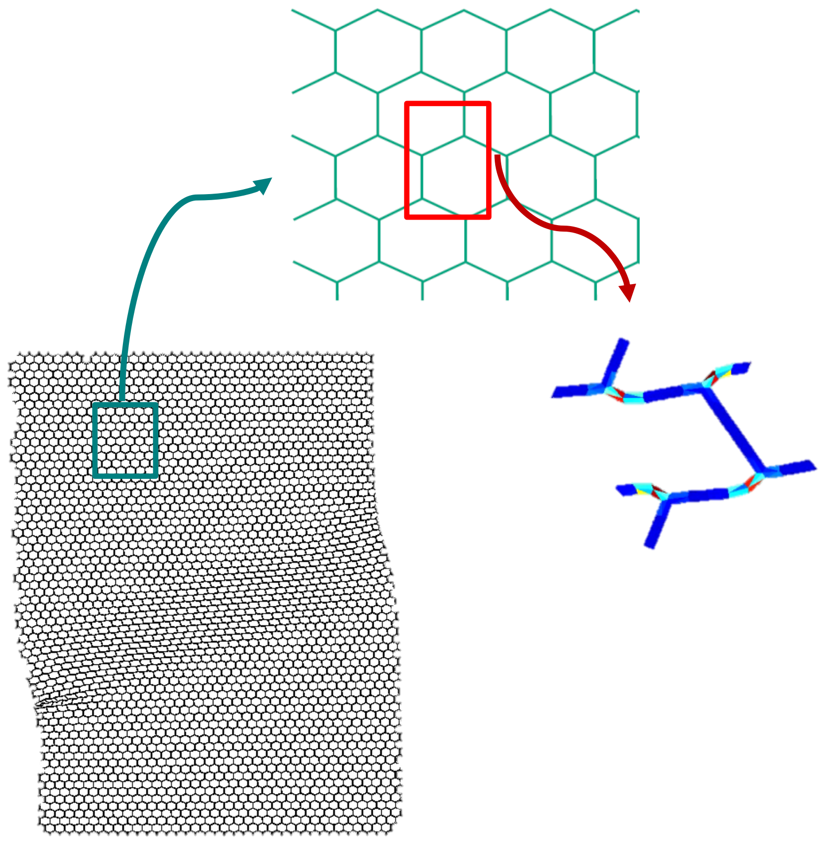
      ⇨ How can we recover the solution unicity at the macro-scale?
  - Macro-scale
    - Localization bands

      ⇨ How to remain computationally efficient

      ⇨ How to capture the instability?

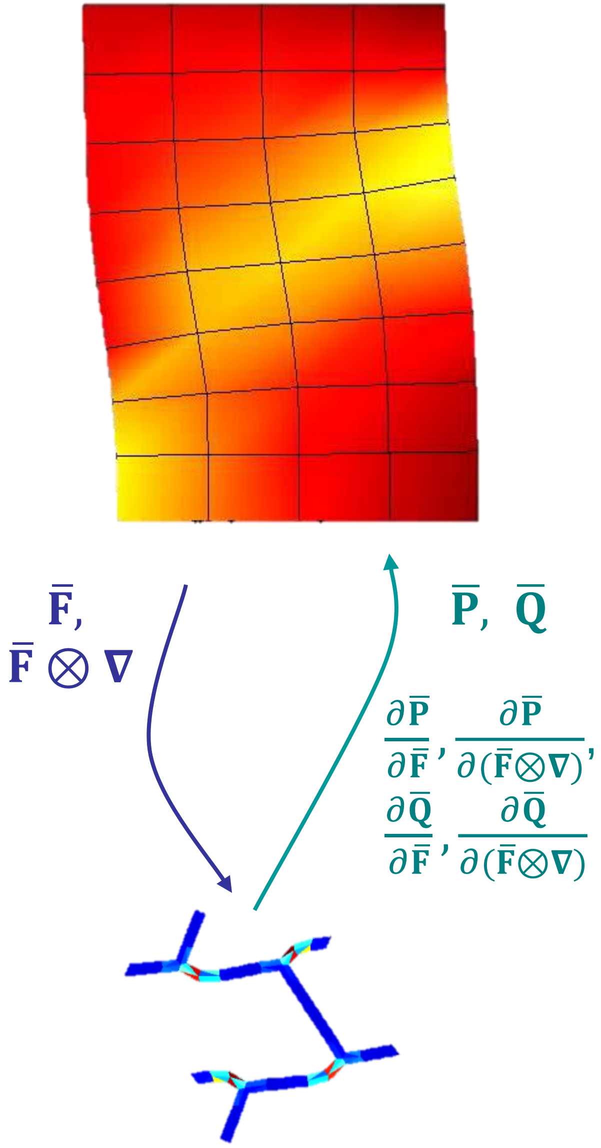


- Recover solution unicity: second-order FE²
  - Macro-scale
    - High-order Strain-Gradient formulation

$$\bar{\mathbf{P}}(\bar{\boldsymbol{X}}) \cdot \boldsymbol{\nabla}_0 - \bar{\mathbf{Q}}(\bar{\boldsymbol{X}}) : (\boldsymbol{\nabla}_0 \otimes \boldsymbol{\nabla}_0) = 0$$

    - Partitioned mesh (//)
  - Transition
    - Gauss points on different processors
    - Each Gauss point is associated to one mesh and one solver
  - Micro-scale
    - Usual continuum

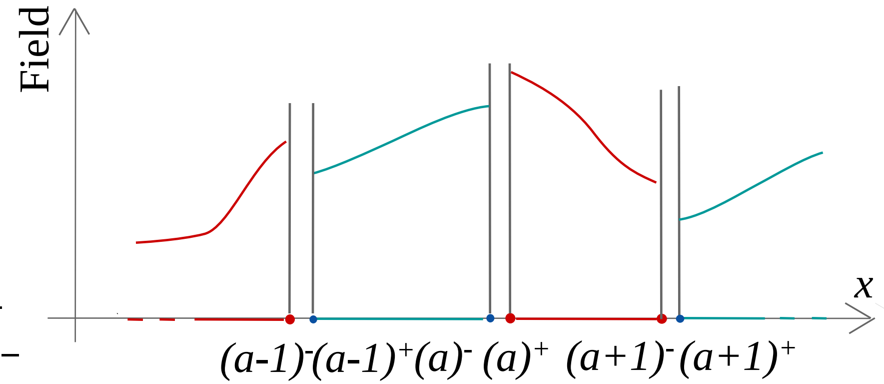
$$\mathbf{P}(\boldsymbol{X}) \cdot \boldsymbol{\nabla}_0 = 0$$




Kouznetsova et al. 2002, Geers et al. 2010, …

# Computational homogenization for foamed materials

- Discontinuous Galerkin (DG) implementation of the second order continuum
  - Finite-element discretization
  - Same **discontinuous** polynomial approximations for the
    - **Test** functions $\varphi_h$ and
    - **Trial** functions $\delta\varphi$
  - Definition of operators on the interface trace:
    - **Jump** operator: $[\![\cdot]\!] = \cdot^{+} - \cdot^{-}$
    - **Mean** operator: $\langle\cdot\rangle = \dfrac{\cdot^{+} + \cdot^{-}}{2}$




  - Continuity is weakly enforced, such that the method
    - Is consistent
    - Is stable
    - Has the optimal convergence rate
  - Can be used to weakly enforce higher discontinuities

- Second-order $FE^2$ method
  - Macro-scale second order continuum

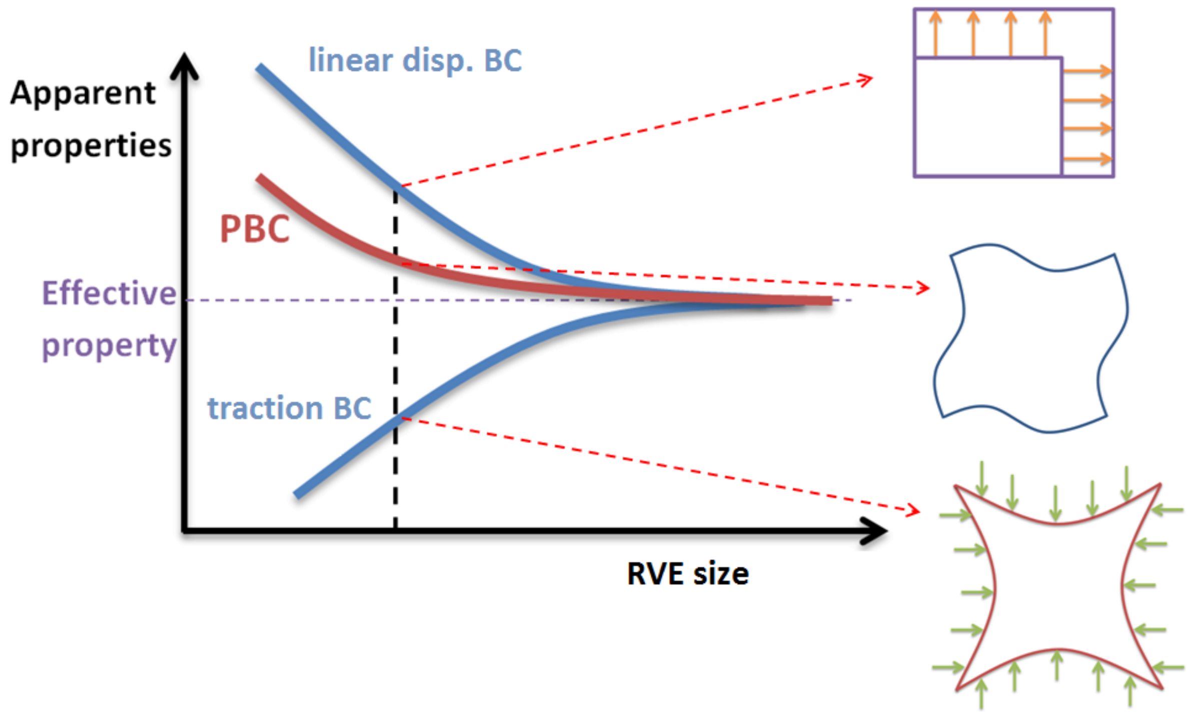
$$\bar{\mathbf{P}}(\bar{\boldsymbol{X}}) \cdot \boldsymbol{\nabla}_0 - \bar{\mathbf{Q}}(\bar{\boldsymbol{X}}) : (\boldsymbol{\nabla}_0 \otimes \boldsymbol{\nabla}_0) = 0$$

  - Requires $\mathbb{C}^1$ shape functions on the mesh
  - The $\mathbb{C}^1$ can be weakly enforced using the DG method

$$a(\bar{\boldsymbol{u}}, \delta\bar{\boldsymbol{u}}) = a^{\text{bulk}}(\bar{\boldsymbol{u}}, \delta\bar{\boldsymbol{u}}) + a^{\text{PI}}(\bar{\boldsymbol{u}}, \delta\bar{\boldsymbol{u}}) + a^{\text{QI}}(\bar{\boldsymbol{u}}, \delta\bar{\boldsymbol{u}}) = b(\delta\bar{\boldsymbol{u}})$$

# Computational homogenization for foamed materials

- Micro-scale periodic boundary conditions
  - Convergence in terms of RVE size




  - Periodic boundary condition is the optimum choice for periodic structures

  - Periodic boundary condition remains interesting for non-periodic structures

# Computational homogenization for foamed materials

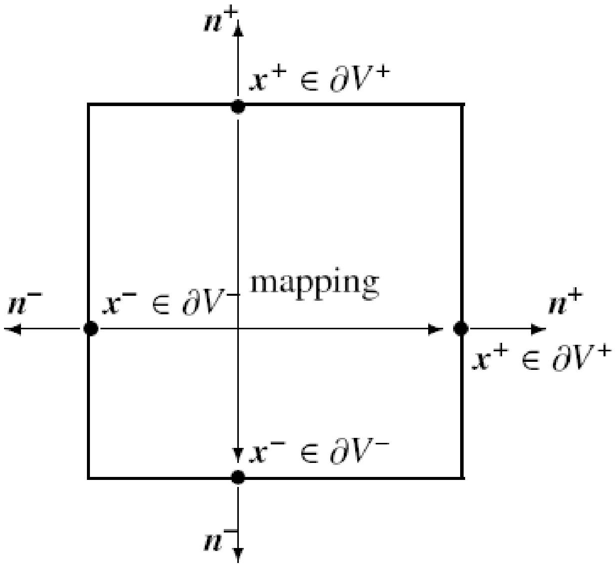
- Micro-scale periodic boundary conditions (2)
  - Defined from the fluctuation field

$$\boldsymbol{w} = \boldsymbol{u} - (\bar{\mathbf{F}} - \mathbf{I}) \cdot \boldsymbol{X} + \frac{1}{2}(\bar{\mathbf{F}} \otimes \boldsymbol{\nabla}_0) : (\boldsymbol{X} \otimes \boldsymbol{X})$$

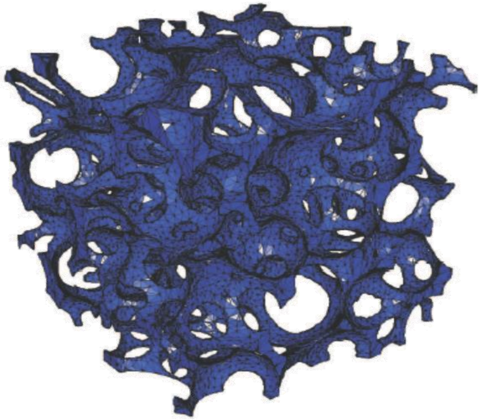
  - Stated on opposite RVE sizes

$$\begin{cases} \boldsymbol{w}(\boldsymbol{X}^+) = \boldsymbol{w}(\boldsymbol{X}^-) \\ \int_{\partial V^-} \boldsymbol{w}(\boldsymbol{X}) d\partial V = \mathbf{0} \end{cases}$$

  - Can be achieved by constraining opposite nodes



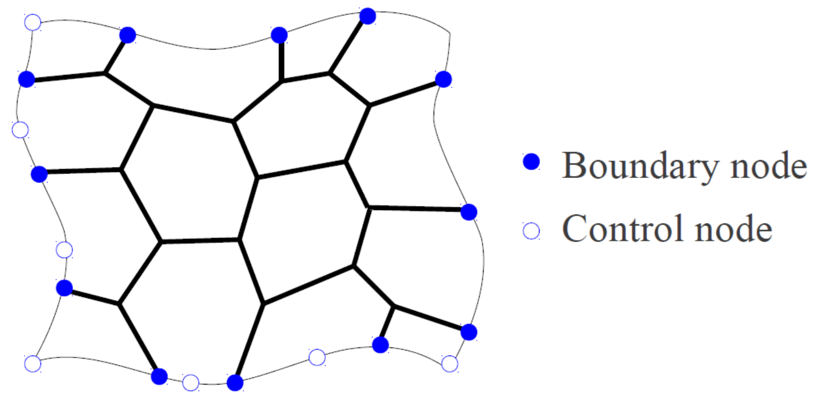

- Foamed materials
  - Usually random meshes
  - Important voids on the boundaries



- Honeycomb structures
  - Not periodic due to the imperfections

- Micro-scale periodic boundary conditions (2)
  - New interpolant method

$$\begin{cases} \boldsymbol{w}(\boldsymbol{X}^-) = \sum_k \mathrm{N}(\boldsymbol{X})\boldsymbol{w}^k \\ \boldsymbol{w}(\boldsymbol{X}^+) = \sum_k \mathrm{N}(\boldsymbol{X})\boldsymbol{w}^k \\ \int_{\partial V^-} \left( \sum_k \mathrm{N}(\boldsymbol{X})\boldsymbol{w}^k \right) d\partial V = \boldsymbol{0} \end{cases}$$




  - Use of Lagrange, cubic spline .. interpolations
  - Fits for
    - Arbitrary meshes
    - Important voids on the RVE sides
  - Results in new constraints in terms of the boundary and control nodes displacements

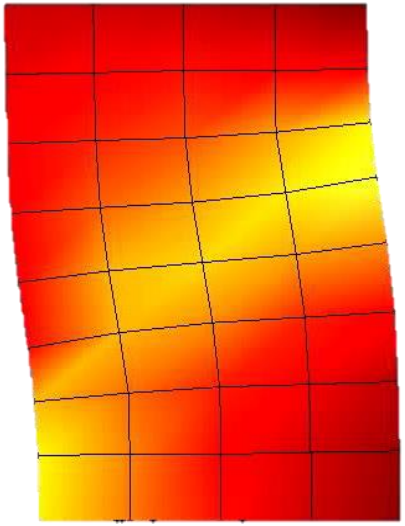
$$\widetilde{\boldsymbol{C}}\,\widetilde{\boldsymbol{u}}_b - \boldsymbol{g}(\overline{\mathbf{F}}, \overline{\mathbf{F}} \otimes \boldsymbol{\nabla}_0) = 0$$

- Capturing instabilities
  - Macro-scale: localization bands
    - Path following method on the applied loading

$$a(\bar{\boldsymbol{u}}, \delta\bar{\boldsymbol{u}}\,) = \bar{\mu}\, b(\delta\bar{\boldsymbol{u}})$$

    - Arc-length constraint on the load increment

$$\bar{h}(\Delta\bar{\boldsymbol{u}}, \Delta\bar{\mu}\,) = \frac{\Delta\bar{\boldsymbol{u}} \cdot \Delta\bar{\boldsymbol{u}}}{\bar{X}_0^2} + \Delta\bar{\mu}^2 - \Delta L^2 = 0$$



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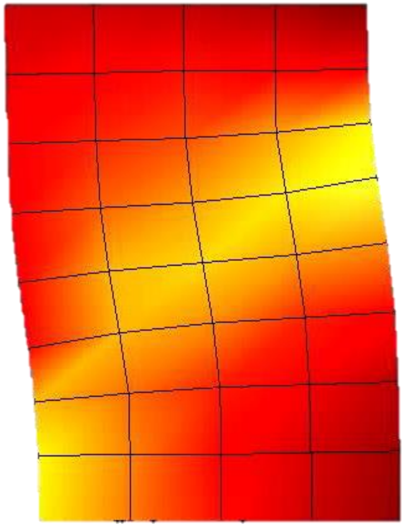

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$\bar{\mathbf{F}}$, $\bar{\mathbf{F}} \otimes \boldsymbol{\nabla}$

$\bar{\mathbf{P}}$, $\bar{\mathbf{Q}}$

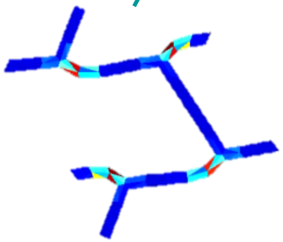
$\frac{\partial\bar{\mathbf{P}}}{\partial\bar{\mathbf{F}}}, \frac{\partial\bar{\mathbf{P}}}{\partial(\bar{\mathbf{F}}\otimes\boldsymbol{\nabla})},$

$\frac{\partial\bar{\mathbf{Q}}}{\partial\bar{\mathbf{F}}}, \frac{\partial\bar{\mathbf{Q}}}{\partial(\bar{\mathbf{F}}\otimes\boldsymbol{\nabla})}$

  - Micro-scale
    - Path following method on the applied boundary conditions

$$\widetilde{\boldsymbol{C}}\, \widetilde{\boldsymbol{u}}_b - \boldsymbol{g}(\bar{\mathbf{F}}, \bar{\mathbf{F}} \otimes \boldsymbol{\nabla}_0) = 0$$

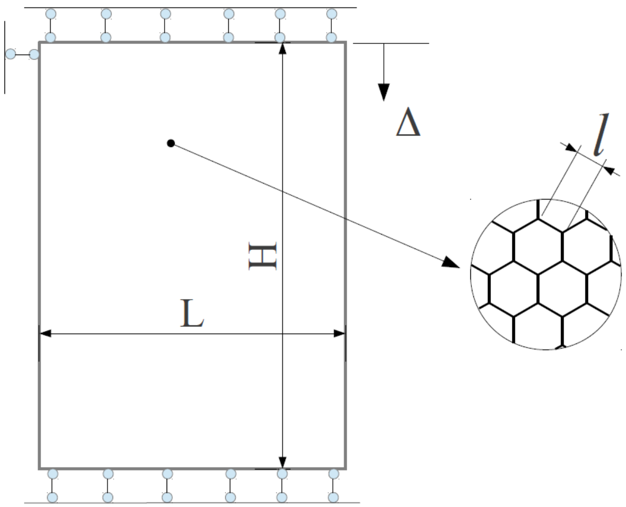
$$\begin{cases} \bar{\mathbf{F}} = \bar{\mathbf{F}}_0 + \mu\, \Delta\bar{\mathbf{F}} \\ \bar{\mathbf{F}} \otimes \boldsymbol{\nabla}_0 = (\bar{\mathbf{F}} \otimes \boldsymbol{\nabla}_0)_0 + \mu\, \Delta(\bar{\mathbf{F}} \otimes \boldsymbol{\nabla}_0) \end{cases}$$



    - Arc-length constraint on the load increment

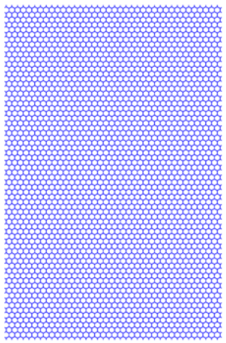
$$h(\Delta\boldsymbol{u}, \Delta\mu) = \frac{\Delta\boldsymbol{u} \cdot \Delta\boldsymbol{u}}{X_0^2} + \Delta\mu^2 - \Delta l^2 = 0$$

- Compression of an hexagonal honeycomb
  - Elasto-plastic material

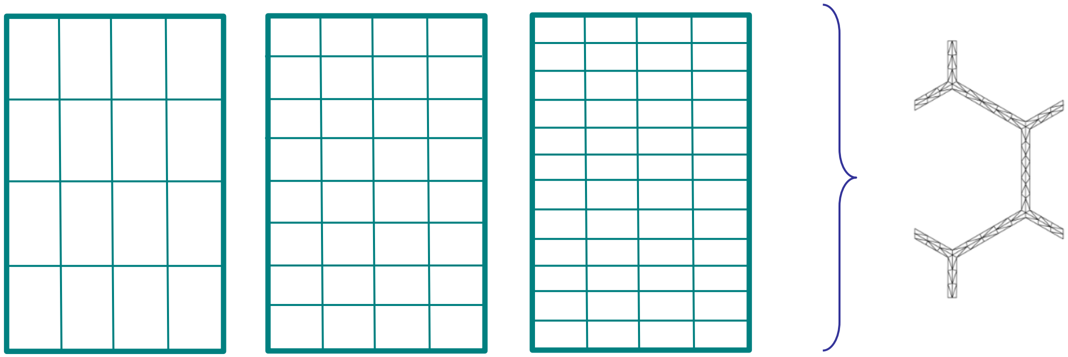



- Comparison of different solutions

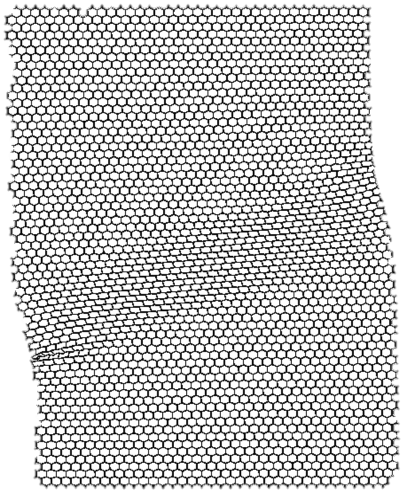
Full direct simulation

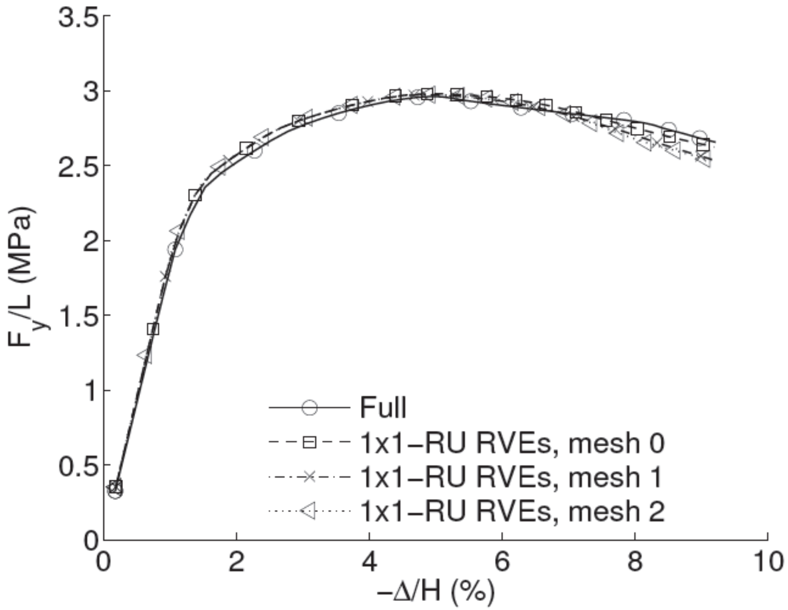


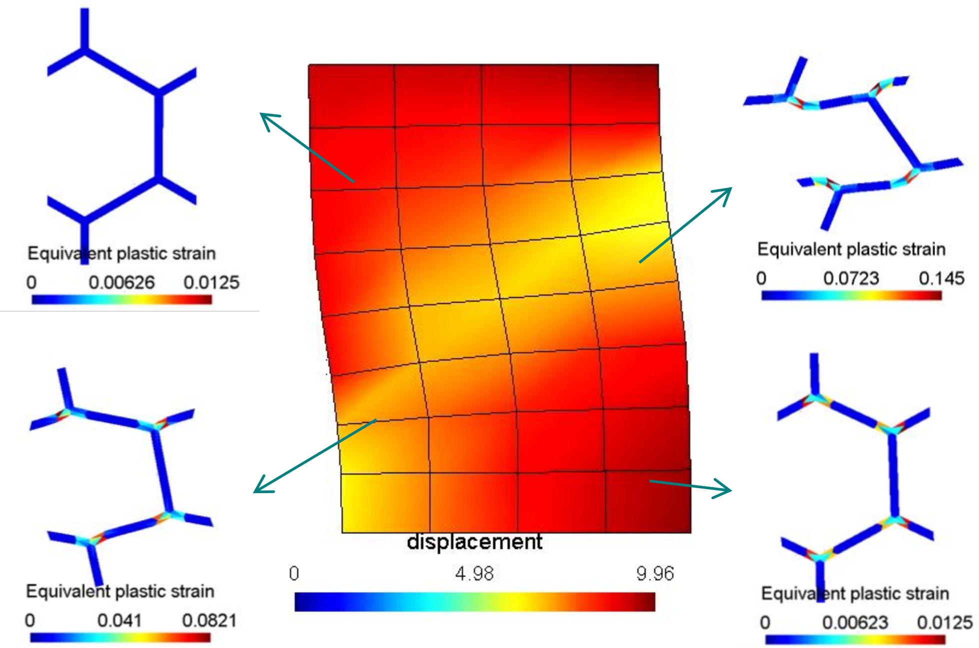
Multiscale with different macro-meshes



- Compression of an hexagonal honeycomb (2)
  - Captures the softening onset
  - Captures the softening response
  - No macro-mesh size effect

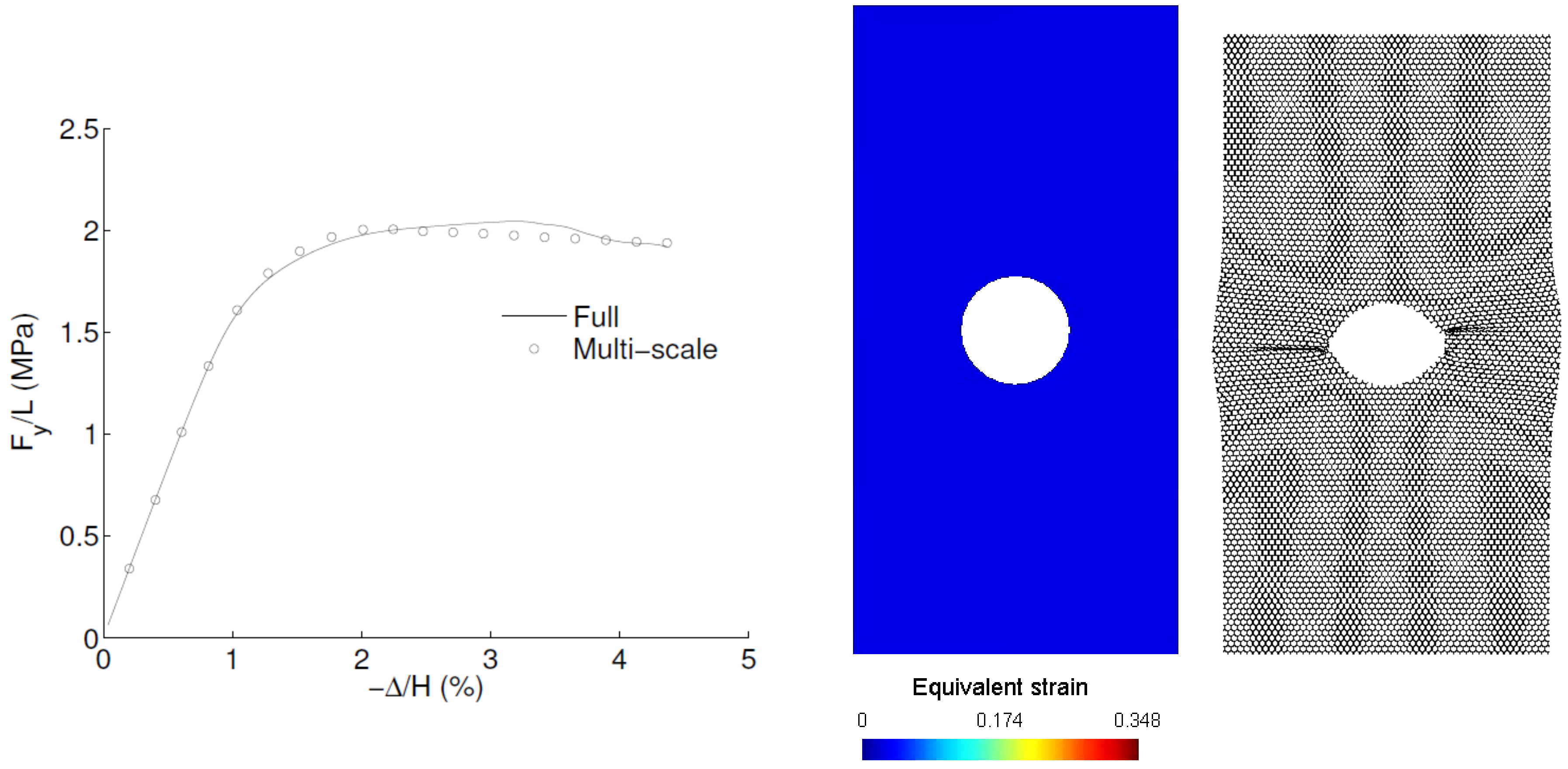




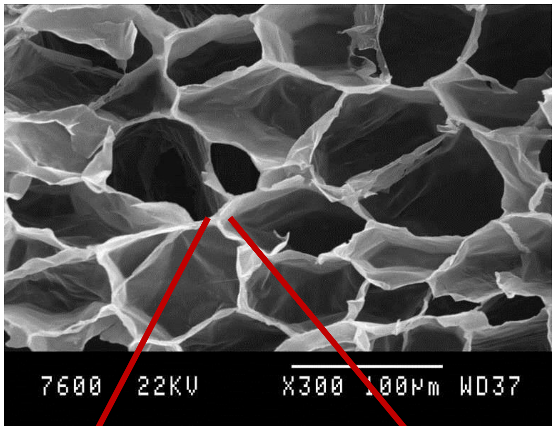
# Computational homogenization for foamed materials

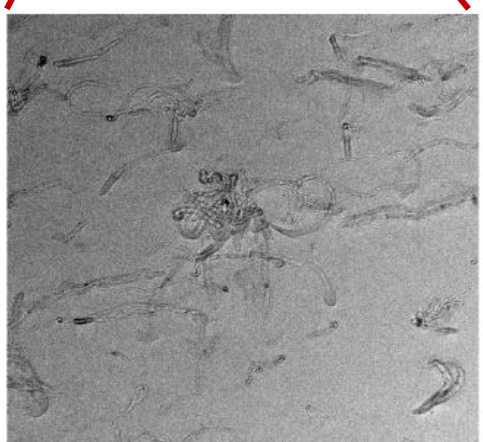
- Compression of an hexagonal honeycomb plate with a centered hole
  - Results given by full and multi-scale models are comparable



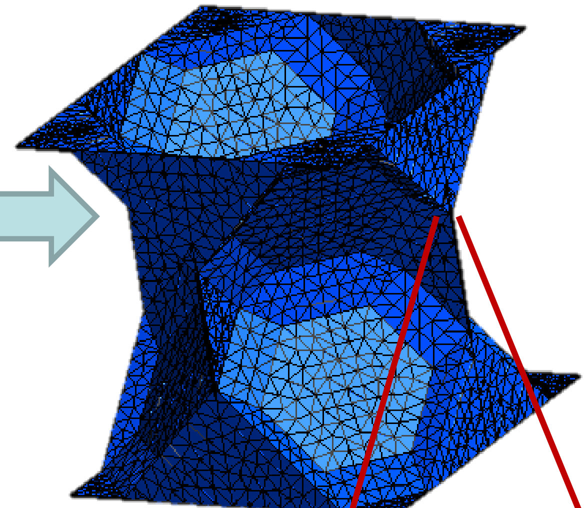
- Carbon-nanotubes-reinforced PolyPropylene foam

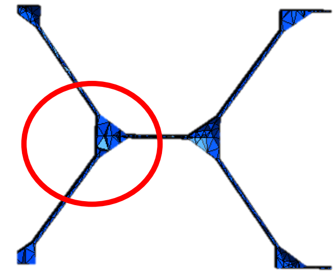
Foamed PP/CNTs



Tetrakaidecahedron with mass concentration

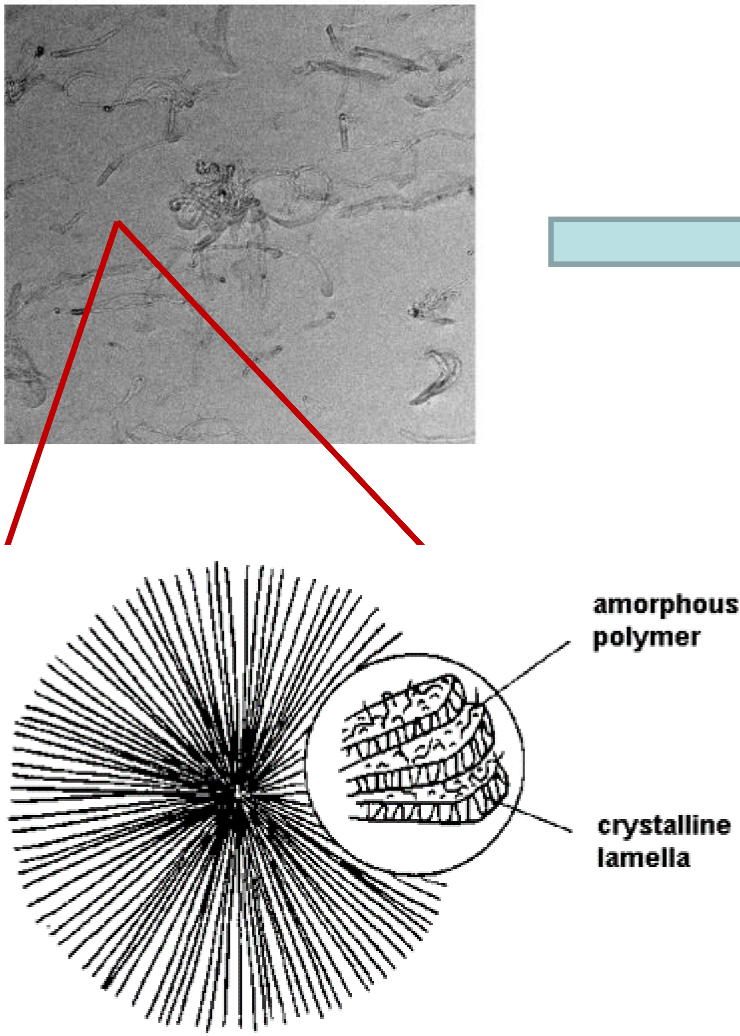




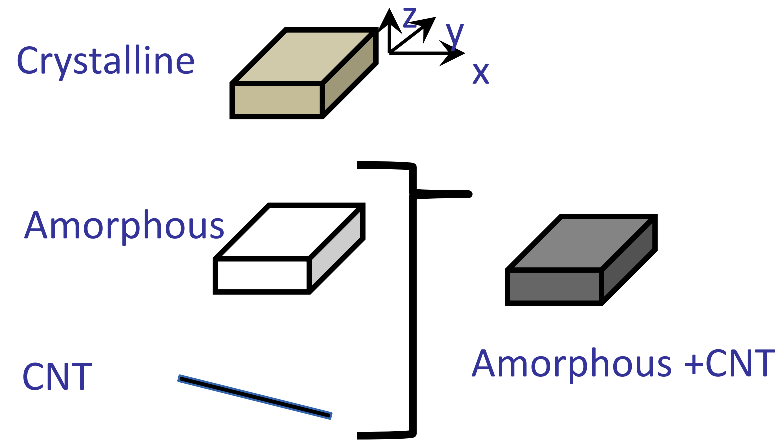
?

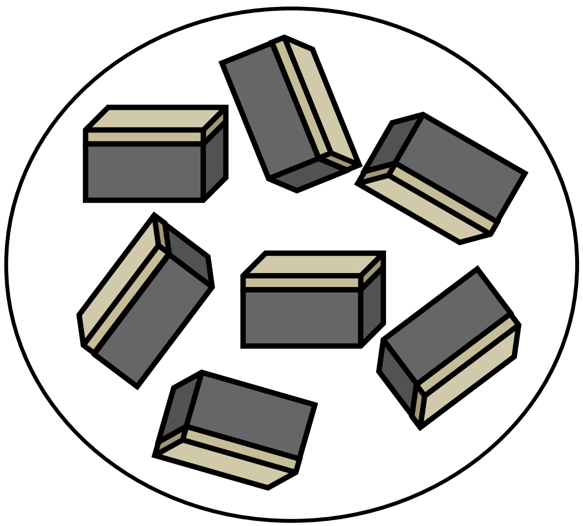
- Carbon-nanotubes-reinforced Polypropylene foam (2)

PP/CNTs composite



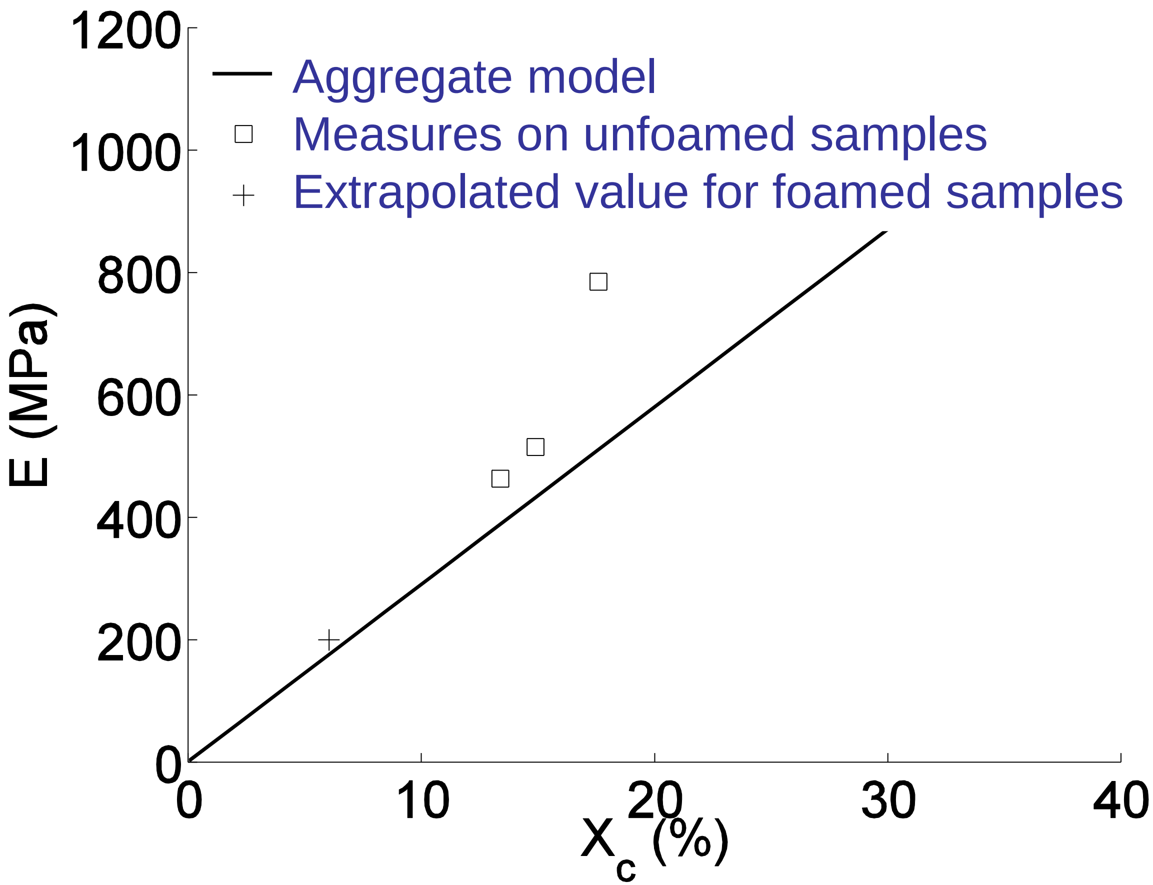

Aggregate model



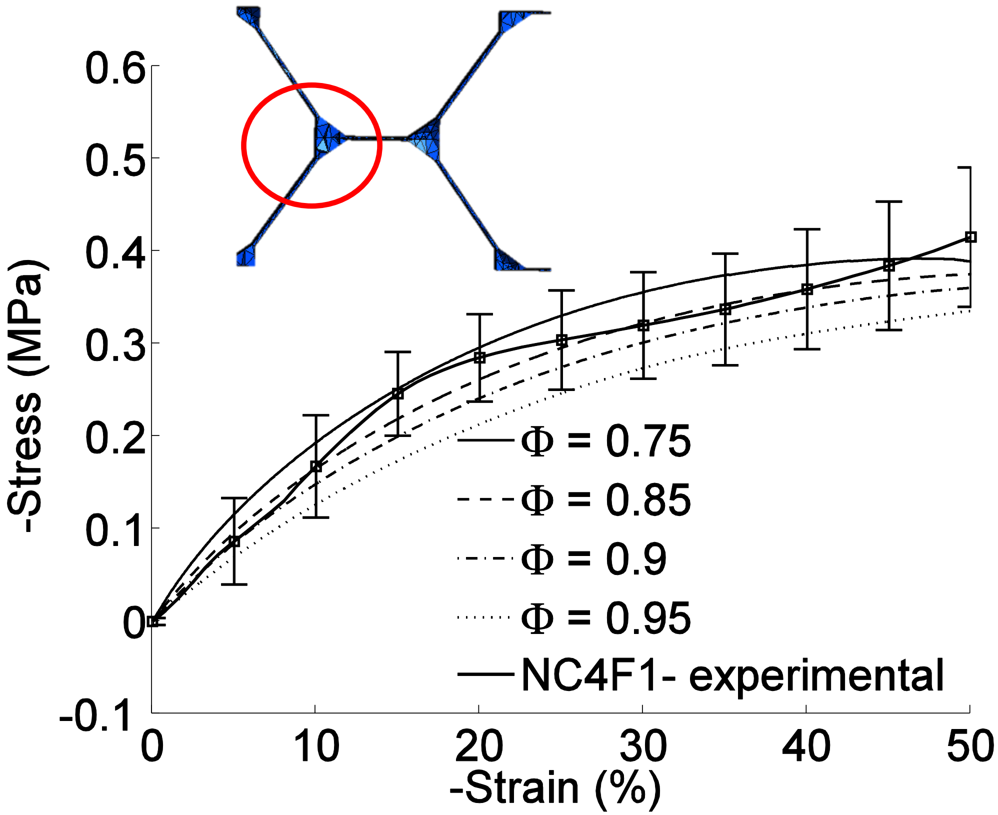



# Validation

- PP/CNTs composite material properties
  - Crystallinity degree from Differential Scanning Calorimetry
    - Different for foamed and unfoamed materials
    - Aggregate model (mean-field homogenization) predictions



- Compressive tests on the foamed samples
  - Dependence on the mass parameter $\Phi$



# Conclusions

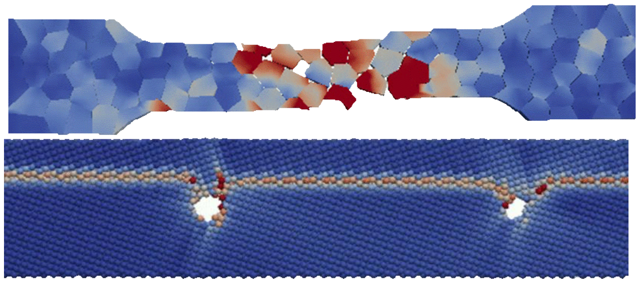
- Computational homogenization for foamed materials
  - Second-order $FE^2$ method
  - Micro-buckling propagation
  - General way of enforcing PBC
  - More in
    - 10.1016/j.cma.2013.03.024
    - 10.1016/j.commatsci.2011.10.017
    - 10.1016/j.ijsolstr.2014.02.029
- Validation on PP/CNTs foamed materials
- Open-source software
  - Implemented in GMSH
    - http://geuz.org/gmsh/

# Computational & Multiscale Mechanics of Materials

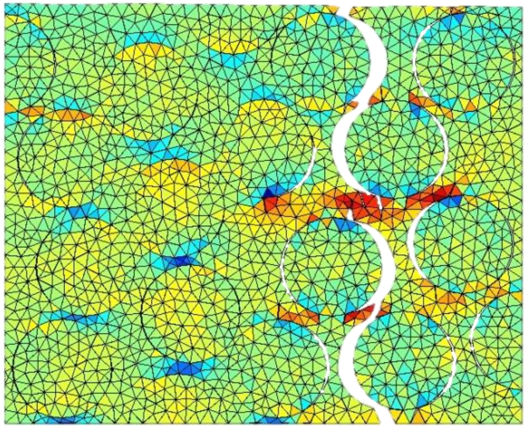
# CM3

www.ltas-cm3.ulg.ac.be

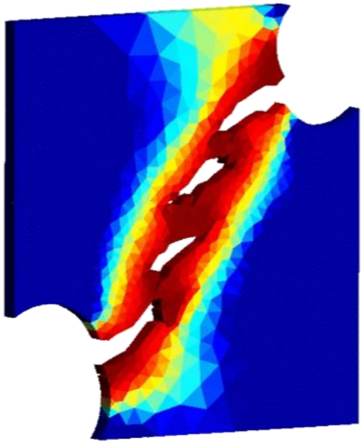
Ludovic Noels, G. Becker,
L. Homsi, V. Lucas, S. Mulay,
V.-D. Nguyen, V. Péron-Lührs,
V.-H. Truong, F. Wan, L. Wu



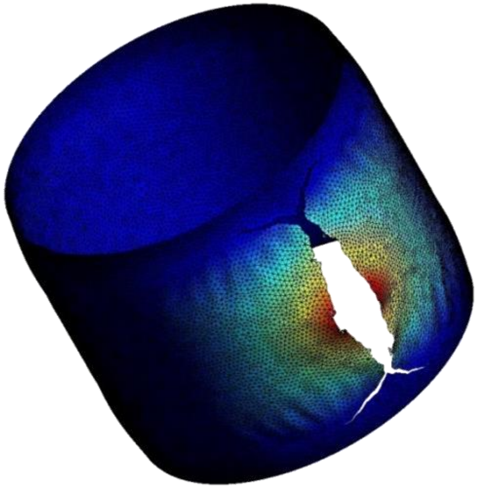
QC method for grain-boundary sliding



DG-based fracture framework



Damage to crack transition



DG-based fracture framework

SVE size effect on meso-scale properties