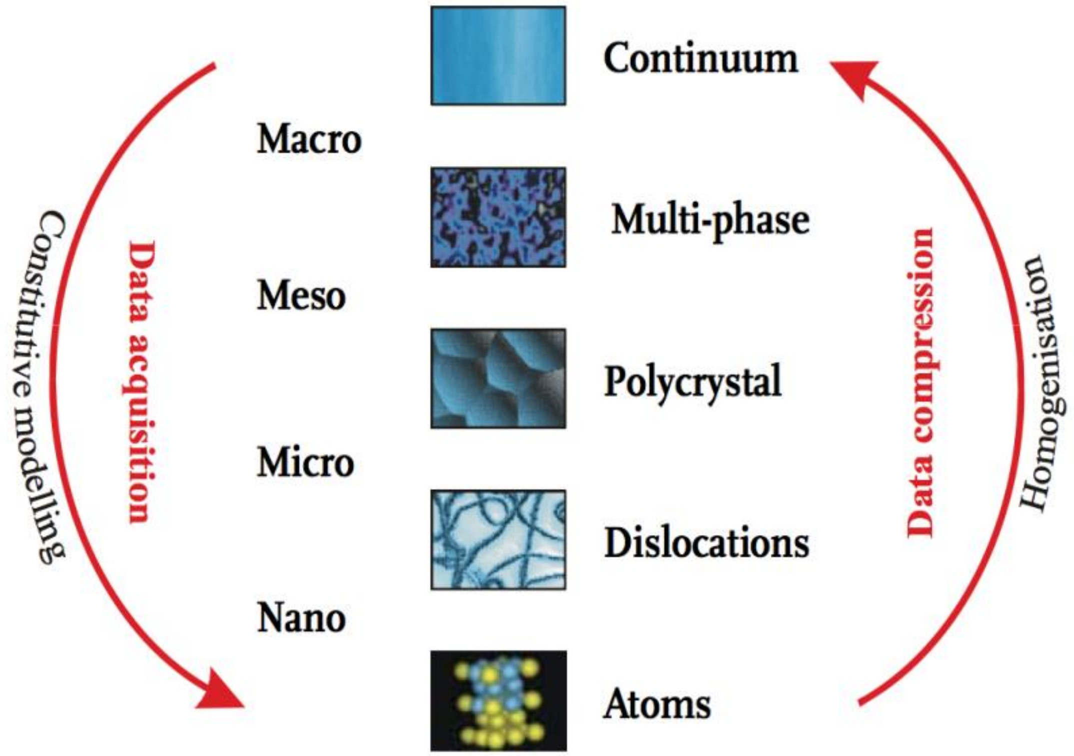
Multiscale studies of foamed materials

V. D. NGUYEN & L. Noels
LTAS-CM3, University of Liège

COMPLAS XII – Barcelona – September 3-5, 2013

Introduction

- Materials are heterogeneous in nature

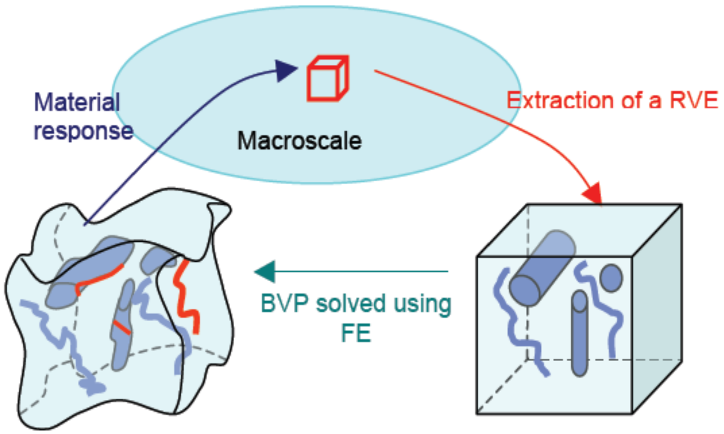


Introduction

- Study of foamed materials by finite element method
  - Full approach
    - Consider the details of the microstructure
    - Lead to an enormous number of unknowns
    - Suitable for problems with limited sizes
  - Macroscopic approach
    - Consider structure as a continuum media
    - Use a phenomenological material law
    - Difficult and expensive to measure material parameters
    - Cannot observe the details of the microstructure during loading
  - Multi—scale computational homogenization (MCH) approach (also—called FE2)
    - Combine the two approaches

Introduction

- MCH approach
  - Macro—scale: a continuum mechanics problem is considered
  - At a macroscopic material point, the material properties are extracted from the solution of a representative volume element (RVE) of the microstructure



  - First—order scheme
    - Macroscopic classical continuum

$$\bar{\mathbf{P}} \cdot \boldsymbol{\nabla} = \mathbf{0}$$

  - Second—order scheme
    - Macroscopic generalized continuum: Mindlin strain gradient, Cosserat, etc.

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

Introduction

- Complex behavior of foamed material
  - Localization due to micro—buckling at thin components (cell edge, cell struts, etc.)
    - Loss of uniqueness
  - Size effects
    - Cell size

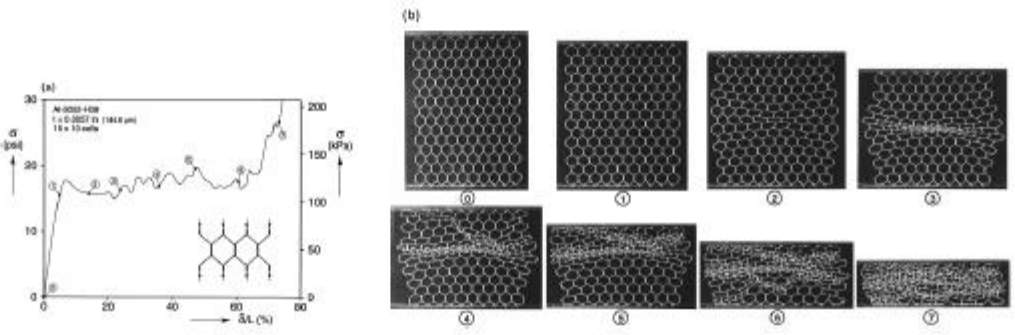


Figure: Force-displacement crushing response of polycarbonate honeycomb - S. D. Papka and S. Kyriakides (1999)

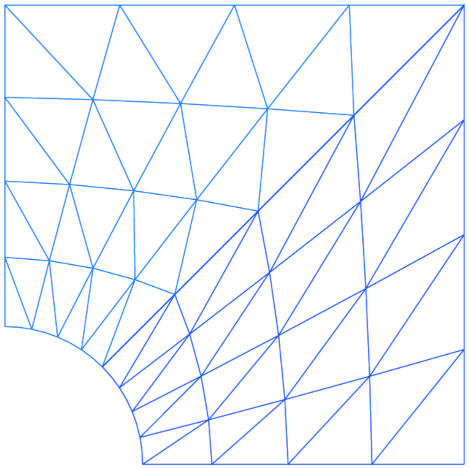
→Motivate the use of second—order MCH (proposed by Kouzenetsova et al. 2004)

Outline

- Second—order multiscale computational homogenization
- Macro—scale : Discontinuous Galerkin method for solving Mindlin strain gradient continuum
- Micro—scale: Polynomial interpolation method for imposing periodic boundary condition
- Path following for macroscopic and microscopic problems
- Numerical examples

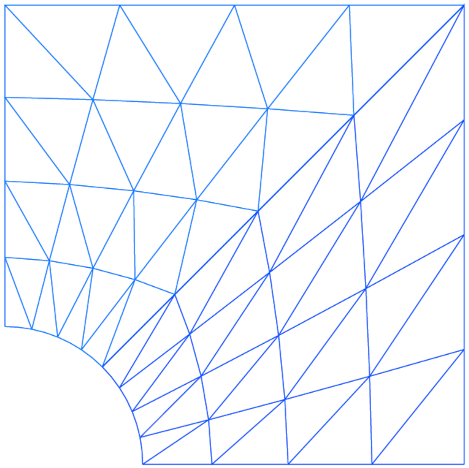
Second—order MCH

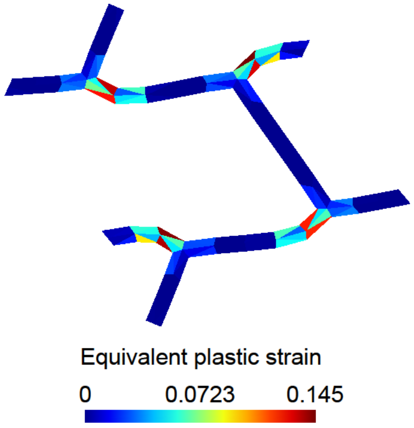
- Macroscopic Mindlin strain gradient continuum
  - At each macroscopic GP, $\bar{\mathbf{F}}$ and $\bar{\mathbf{G}} = \bar{\mathbf{F}} \otimes \boldsymbol{\nabla}$ are known. $\bar{\mathbf{P}}$, $\bar{\mathbf{Q}}$ are sought.



Second—order MCH

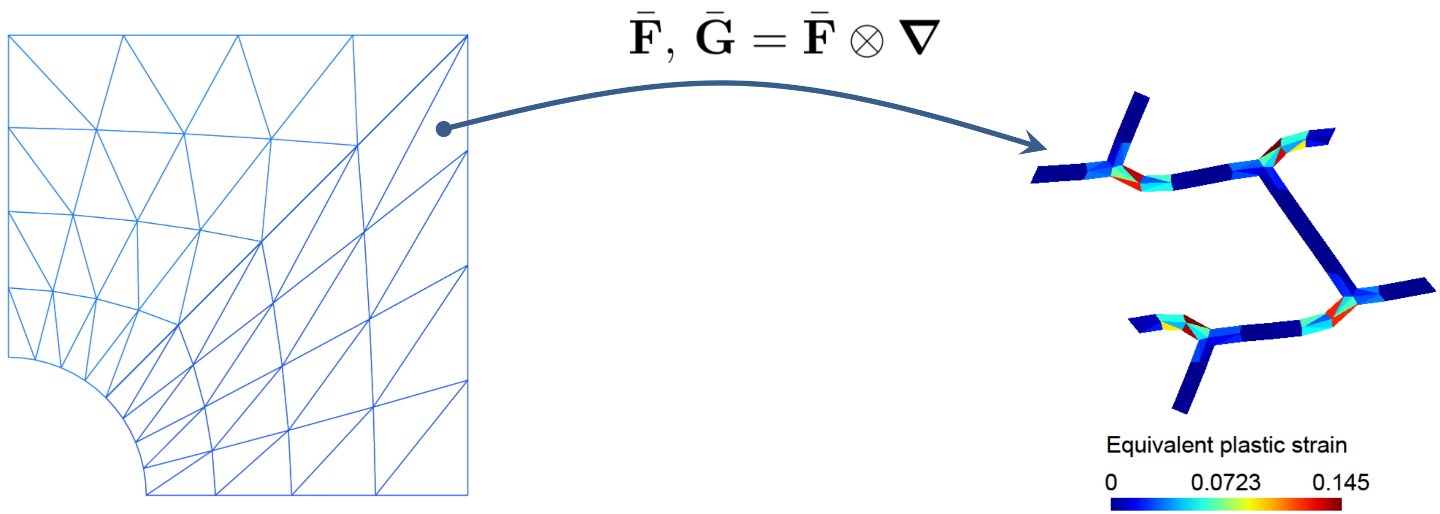
- Microscopic classical continuum with periodic boundary condition (PBC)
  - Usual 3D finite elements
  - Second—order PBC





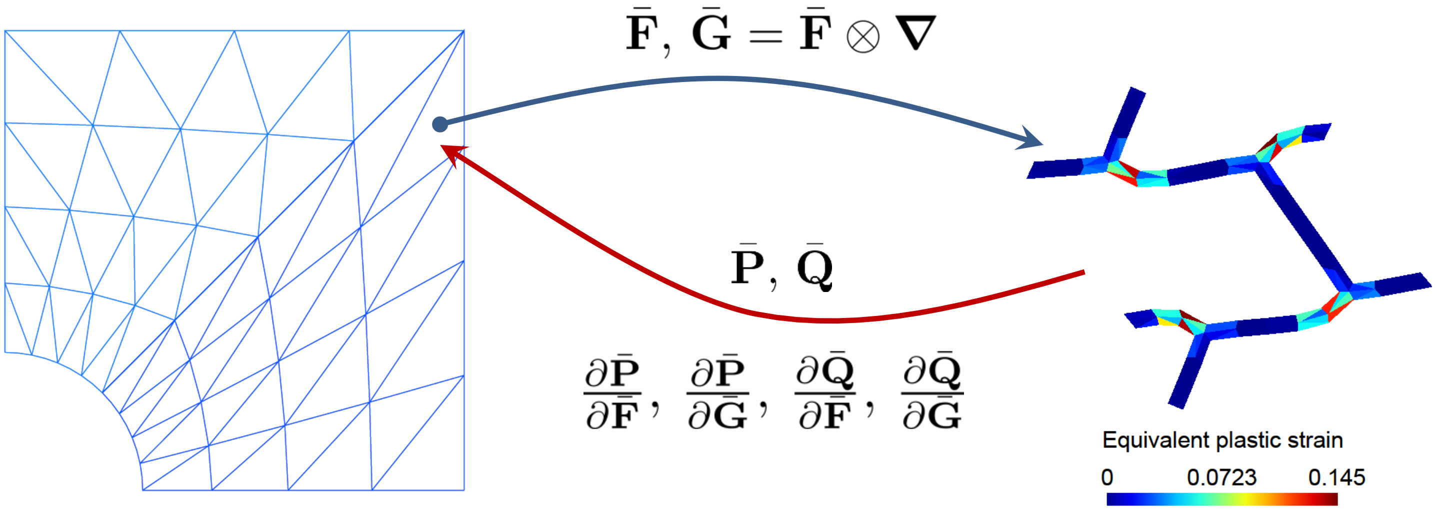
Second—order MCH

- Scale transition
  - **Downscaling**: $\bar{\mathbf{F}}$ and $\bar{\mathbf{G}} = \bar{\mathbf{F}} \otimes \boldsymbol{\nabla}$ are used to define the microscopic BCs



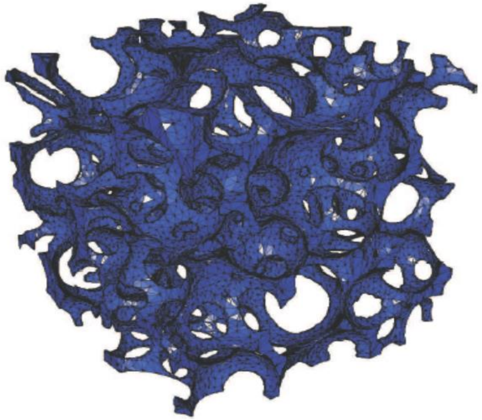
Second—order MCH

- Scale transition
  - **Downscaling**: $\bar{\mathbf{F}}$ and $\bar{\mathbf{G}} = \bar{\mathbf{F}} \otimes \boldsymbol{\nabla}$ are used to define the microscopic BCs
  - **Upscaling**: $\bar{\mathbf{P}}$, $\bar{\mathbf{Q}}$ and 4 tangent operators are extracted from the solution of the microscopic boundary value problem



Second—order MCH for foamed materials

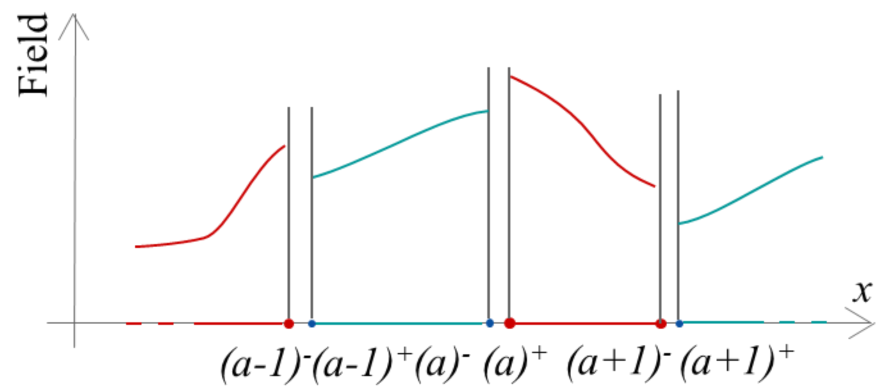
- Macroscopic Mindlin strain gradient continuum
  - Require the continuities of displacement and of its derivatives
  - Use the discontinuous Galerkin (DG) method
- High—order PBC
  - General non—conforming meshes because of random spatial distribution
  - Use the polynomial interpolation method
- Instabilities
  - Use the path following method at both scales



RVE of random foam

Macro—scale: DG method

- Finite element discretization
- Same discontinuous polynomial approximations for the test and trial functions
- Definition of interface operators
  - Jump operator: $[\![\cdot]\!] = \cdot^{+} - \cdot^{-}$
  - Mean operator: $\langle\cdot\rangle = \frac{\cdot^{+} + \cdot^{-}}{2}$
- Continuity is weakly enforced



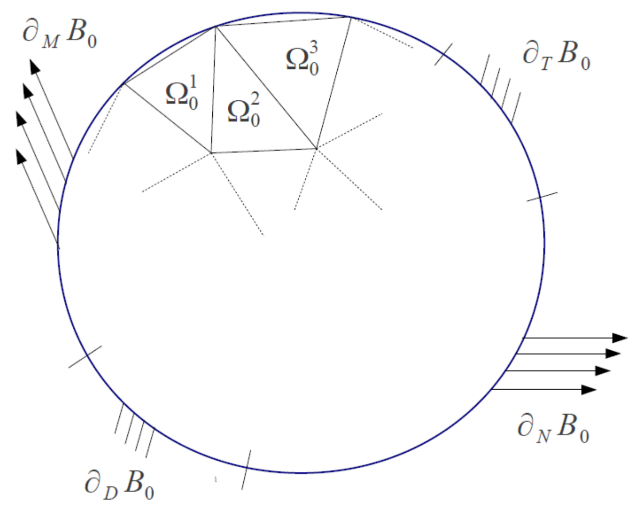
Macro—scale: DG method

- Mindlin strain gradient continuum
  - Strong form in terms of first Piola—Kirchoff stress $\bar{\mathbf{P}}$ and higher—order stress $\bar{\mathbf{Q}}$ (conjugate with deformation gradient $\bar{\mathbf{F}}$ and its gradient $\bar{\mathbf{G}}$)

$$\bar{\mathbf{P}}\left(\bar{\mathbf{X}}\right)\cdot\boldsymbol{\nabla}_0-\bar{\mathbf{Q}}\left(\bar{\mathbf{X}}\right):\left(\boldsymbol{\nabla}_0\otimes\boldsymbol{\nabla}_0\right)=\mathbf{0}\quad\forall\bar{\mathbf{X}}\in B_0$$

  - Boundary conditions

$$\begin{cases}\bar{\mathbf{u}}=\bar{\mathbf{u}}^0 & \forall\bar{\mathbf{X}}\in\partial_D B_0\\ \bar{\mathbf{T}}=\bar{\mu}\bar{\mathbf{T}}^0 & \forall\bar{\mathbf{X}}\in\partial_N B_0\\ \mathrm{D}\bar{\mathbf{u}}=\mathrm{D}\bar{\mathbf{u}}^0 & \forall\bar{\mathbf{X}}\in\partial_T B_0\\ \bar{\mathbf{R}}=\bar{\mu}\bar{\mathbf{R}}^0 & \forall\bar{\mathbf{X}}\in\partial_M B_0\end{cases}$$



  - Definitions

$$\bar{\mathbf{T}}=\left(\bar{\mathbf{P}}-\bar{\mathbf{Q}}\cdot\boldsymbol{\nabla}_0\right)\cdot\bar{\mathbf{N}}+\left(\mathbf{Q}\cdot\bar{\mathbf{N}}\right)\cdot\left(\bar{\mathbf{N}}\,\overset{s}{\boldsymbol{\nabla}}_0\cdot\bar{\mathbf{N}}-\overset{s}{\boldsymbol{\nabla}}_0\right)\qquad \mathrm{D}=\bar{\mathbf{N}}\cdot\boldsymbol{\nabla}_0\,,$$

$$\bar{\mathbf{R}}=\bar{\mathbf{Q}}:\left(\bar{\mathbf{N}}\otimes\bar{\mathbf{N}}\right)\qquad \overset{s}{\boldsymbol{\nabla}}_0=\left(\mathbf{I}-\bar{\mathbf{N}}\otimes\bar{\mathbf{N}}\right)\cdot\boldsymbol{\nabla}_0$$

Macro—scale: DG method

- DG weak form is stated as finding $\bar{\mathbf{u}}$ such that

$$\mathrm{a}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \mathrm{b}\left(\delta\bar{\mathbf{u}}\right) \qquad \forall \delta\bar{\mathbf{u}}$$

  - With

$$\mathrm{a}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \mathrm{a}^{\mathrm{bulk}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) + \mathrm{a}^{\mathrm{PI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) + \mathrm{a}^{\mathrm{QI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right)$$

$$\mathrm{b}\left(\delta\bar{\mathbf{u}}\right) = \bar{\mu}\left(\int_{\partial_N B_0} \bar{\mathbf{T}}^0 \cdot \delta\bar{\mathbf{u}}\, d\partial B + \int_{\partial_M B_0} \bar{\mathbf{R}}^0 \cdot \mathrm{D}\delta\bar{\mathbf{u}}\, d\partial B\right)$$

  - Bulk term

$$\mathrm{a}^{\mathrm{bulk}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \int_{B_0} \left[\bar{\mathbf{P}}\left(\bar{\mathbf{u}}\right) : \bar{\mathbf{F}}\left(\delta\bar{\mathbf{u}}\right) + \bar{\mathbf{Q}}\left(\bar{\mathbf{u}}\right) \vdots \bar{\mathbf{G}}\left(\delta\bar{\mathbf{u}}\right)\right] dB$$

Macro—scale: DG method

- DG weak form is stated as finding $\bar{\mathbf{u}}$ such that

$$\mathrm{a}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \mathrm{b}\left(\delta\bar{\mathbf{u}}\right) \qquad \forall \delta\bar{\mathbf{u}}$$

  – With

$$\mathrm{a}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \mathrm{a}^{\mathrm{bulk}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) + \mathrm{a}^{\mathrm{PI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) + \mathrm{a}^{\mathrm{QI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right)$$

$$\mathrm{b}\left(\delta\bar{\mathbf{u}}\right) = \bar{\mu}\left(\int_{\partial_N B_0} \bar{\mathbf{T}}^0 \cdot \delta\bar{\mathbf{u}} \, d\partial B + \int_{\partial_M B_0} \bar{\mathbf{R}}^0 \cdot \mathrm{D}\delta\bar{\mathbf{u}} \, d\partial B\right)$$

  – First –order interface term

$$\mathrm{a}^{\mathrm{PI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \int_{\partial_I B_0} \Big[[\![\delta\bar{\mathbf{u}}]\!] \cdot \left\langle \hat{\mathbf{P}}\left(\bar{\mathbf{u}}\right)\right\rangle \cdot \bar{\mathbf{N}}^- + [\![\bar{\mathbf{u}}]\!] \cdot \left\langle \hat{\mathbf{P}}\left(\delta\bar{\mathbf{u}}\right)\right\rangle \cdot \bar{\mathbf{N}}^- + [\![\bar{\mathbf{u}}]\!] \otimes \bar{\mathbf{N}}^- : \left\langle \frac{\beta_P}{h_s}\mathbf{C}^0 \right\rangle : [\![\delta\bar{\mathbf{u}}]\!] \otimes \bar{\mathbf{N}}^- \Big] \, d\partial B \,,$$

  – Ensure continuity, consistency and stability of displacement field

Macro—scale: DG method

- DG weak form is stated as finding $\bar{\mathbf{u}}$ such that

$$\mathrm{a}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \mathrm{b}\left(\delta\bar{\mathbf{u}}\right) \qquad \forall \delta\bar{\mathbf{u}}$$

  - With

$$\mathrm{a}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \mathrm{a}^{\mathrm{bulk}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) + \mathrm{a}^{\mathrm{PI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) + \mathrm{a}^{\mathrm{QI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right)$$

$$\mathrm{b}\left(\delta\bar{\mathbf{u}}\right) = \bar{\mu}\left(\int_{\partial_N B_0} \bar{\mathbf{T}}^0 \cdot \delta\bar{\mathbf{u}}\, d\partial B + \int_{\partial_M B_0} \bar{\mathbf{R}}^0 \cdot \mathrm{D}\delta\bar{\mathbf{u}}\, d\partial B\right)$$

  - Second–order interface term

$$\mathrm{a}^{\mathrm{QI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \int_{\partial_I B_0} \Big[[\![\delta\bar{\mathbf{u}} \otimes \boldsymbol{\nabla}_0]\!] : \left\langle \bar{\mathbf{Q}}\left(\bar{\mathbf{u}}\right)\right\rangle \cdot \bar{\mathbf{N}}^- + [\![\bar{\mathbf{u}} \otimes \boldsymbol{\nabla}_0]\!] : \left\langle \bar{\mathbf{Q}}\left(\delta\bar{\mathbf{u}}\right)\right\rangle \cdot \bar{\mathbf{N}}^- + [\![\bar{\mathbf{u}} \otimes \boldsymbol{\nabla}_0]\!] \otimes \bar{\mathbf{N}}^- \vdots \left\langle \frac{\beta_Q}{h_s}\mathbf{J}^0\right\rangle \vdots [\![\delta\bar{\mathbf{u}} \otimes \boldsymbol{\nabla}_0]\!] \otimes \bar{\mathbf{N}}^- \Big]\, d\partial B\,.$$

  - Ensure continuity, consistency and stability of displacement derivatives

Macro—scale: DG method

- DG weak form is stated as finding $\bar{\mathbf{u}}$ such that

$$\mathrm{a}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \mathrm{b}\left(\delta\bar{\mathbf{u}}\right) \qquad \forall \delta\bar{\mathbf{u}}$$

  – With

$$\mathrm{a}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) = \mathrm{a}^{\mathrm{bulk}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) + \mathrm{a}^{\mathrm{PI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right) + \mathrm{a}^{\mathrm{QI}}\left(\bar{\mathbf{u}}, \delta\bar{\mathbf{u}}\right)$$

$$\mathrm{b}\left(\delta\bar{\mathbf{u}}\right) = \bar{\mu}\left(\int_{\partial_N B_0} \bar{\mathbf{T}}^0 \cdot \delta\bar{\mathbf{u}}\, d\partial B + \int_{\partial_M B_0} \bar{\mathbf{R}}^0 \cdot \mathrm{D}\delta\bar{\mathbf{u}}\, d\partial B\right)$$

  – Finite element nonlinear equation

$$\bar{\mathbf{f}}_{\mathrm{int}}\left(\bar{\mathbf{u}}\right) - \bar{\mu}\bar{\mathbf{q}} = \mathbf{0}$$

  – Loading control parameter $\bar{\mu}$ for path following method

Micro—scale: Polynomial interpolation

- Microscopic classical BVP
  - Strong form in terms of first Piola—Kirchoff stress

$$\mathbf{P}(\mathbf{X}) \otimes \boldsymbol{\nabla}_0 = \mathbf{0} \quad \forall \mathbf{X} \in V_0$$

  - Fluctuation field

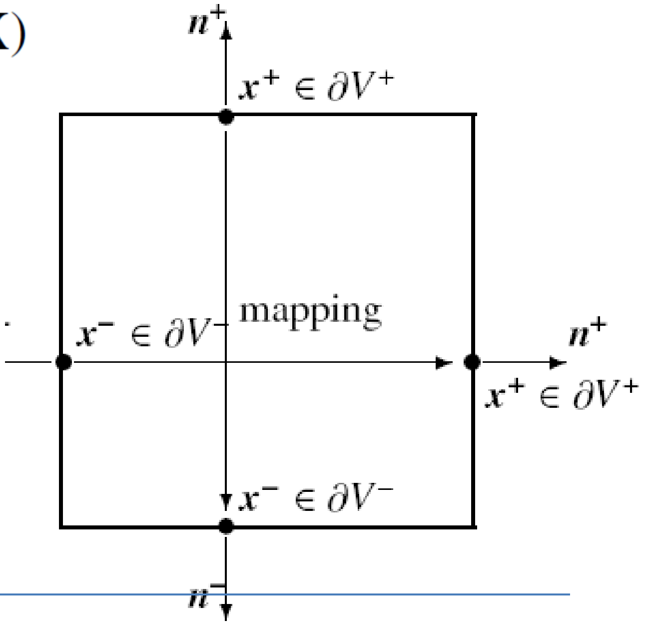
$$\mathbf{w} = \mathbf{u} - \left(\bar{\mathbf{F}} - \mathbf{I}\right) \cdot \mathbf{X} + \frac{1}{2}\bar{\mathbf{G}} : (\mathbf{X} \otimes \mathbf{X})$$

  - Second—order PBC

$$\mathbf{w}(\mathbf{X}^+) = \mathbf{w}(\mathbf{X}^-) \qquad \forall \mathbf{X}^- \in \partial V_0^- \text{ and matching } \mathbf{X}^+ \in \partial V_0^+ .$$

$$\int_{\partial S_i} \mathbf{w}(\mathbf{X})\, d\partial V = \mathbf{0} \quad \forall S_i \subset \partial V^-$$

  - Usually meshes are not conforming



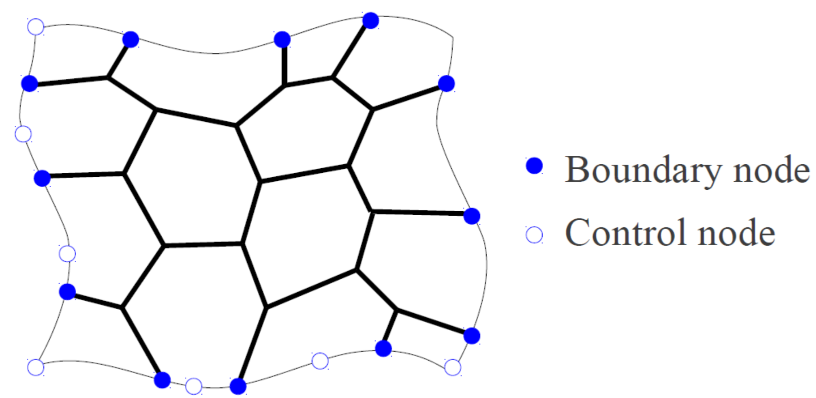
Micro—scale: Polynomial interpolation

- Second—order PBC
  - Control nodes are used to interpolate fluctuation field
    - Lagrange interpolation: use only displacements to interpolate
    - Cubic spline interpolation: use displacements + tangent to interpolate
  - Efficient method when voids are dominant on the boundary
  - Boundary nodes respect to the PBC constraints

$$\mathbf{w}^{-}(\mathbf{X}) = \sum_k \mathbb{N}^k(\mathbf{X})\,\mathbf{w}^k + \sum_k \mathbb{M}^k(\mathbf{X})\,\boldsymbol{\theta}^k ,$$

$$\mathbf{w}^{+}(\mathbf{X}) = \sum_k \mathbb{N}^k(\mathbf{X})\,\mathbf{w}^k + \sum_k \mathbb{M}^k(\mathbf{X})\,\boldsymbol{\theta}^k \text{ and}$$

$$\int_{S\subset\partial V^-}\left(\sum_k \mathbb{N}_k(\mathbf{X})\,\mathbf{w}^k + \sum_k \mathbb{M}^k(\mathbf{X})\,\boldsymbol{\theta}^k\right) d\partial V = \mathbf{0}$$



  - Lead to a linear constraint in terms of displacement $\tilde{\mathbf{C}}\tilde{\mathbf{u}}_b - \mathbf{g}\left(\bar{\mathbf{F}},\bar{\mathbf{G}}\right) = \mathbf{0}$

Micro—scale: Polynomial interpolation

- Second—order PBC
  - Linear constraint in terms of displacement $\tilde{\mathbf{C}}\tilde{\mathbf{u}}_b - \mathbf{g}\left(\bar{\mathbf{F}}, \bar{\mathbf{G}}\right) = \mathbf{0}$
  - Parameterization by a scalar

$$\begin{aligned}\bar{\mathbf{F}}(\mu) &= \bar{\mathbf{F}}_0 + \mu\left(\bar{\mathbf{F}}_1 - \bar{\mathbf{F}}_0\right) = \bar{\mathbf{F}}_0 + \mu\Delta\bar{\mathbf{F}} \text{ and} \\ \bar{\mathbf{G}}(\mu) &= \bar{\mathbf{G}}_0 + \mu\left(\bar{\mathbf{G}}_1 - \bar{\mathbf{G}}_0\right) = \bar{\mathbf{G}}_0 + \mu\Delta\bar{\mathbf{G}},\end{aligned}$$

  - Linear constraint with a scalar

$$\mathbf{Cu} - \mathbf{g}_0 - \mathbf{q}\mu = \mathbf{0}$$

  - Microscopic boundary value problem with linear constraints and Lagrange multipliers

$$\mathbf{f}_{\text{int}}(\mathbf{u}) - \mathbf{C}^T\lambda = \mathbf{0}$$

$$\mathbf{Cu} - \mathbf{g}_0 - \mathbf{q}\mu = \mathbf{0}$$

  - Loading control parameter μ for path following method

Path following method

- Macroscopic path following equation with arc—length increment
  - Nonlinear form

$$\bar{\mathbf{f}}_{\text{int}}(\bar{\mathbf{u}}) - \bar{\mu}\bar{\mathbf{q}} = \mathbf{0}$$

  - Arc—length constraint

$$\bar{h}(\Delta\bar{\mathbf{u}}, \Delta\bar{\mu}) = \frac{\Delta\bar{\mathbf{u}}^T \Delta\bar{\mathbf{u}}}{\Psi^2} + \Delta\bar{\mu}^2 - \Delta L^2 = 0\,,$$

- Macroscopic path following equation with arc—length increment
  - Non—linear form with linear constraints

$$\mathbf{f}_{\text{int}}(\mathbf{u}) - \mathbf{C}^T\lambda = \mathbf{0}$$

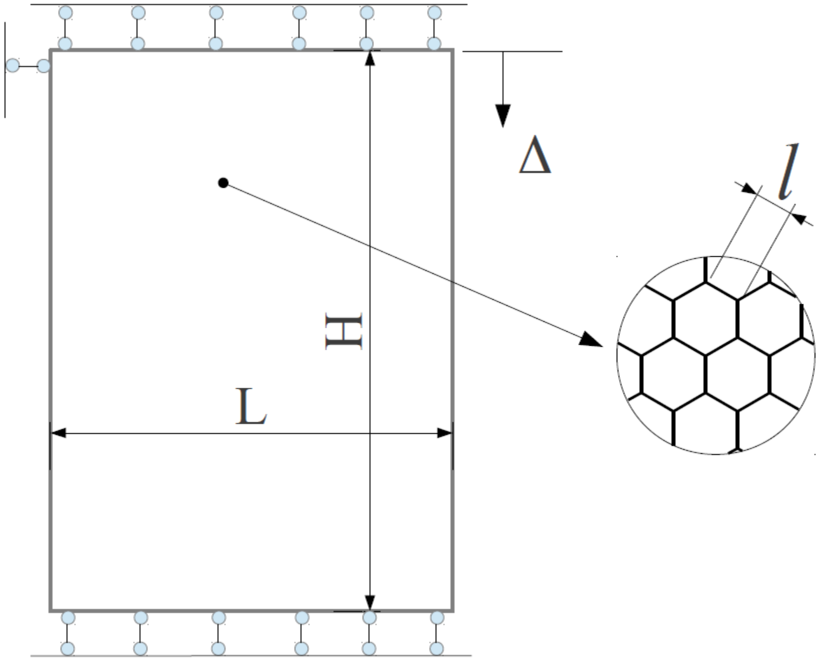
$$\mathbf{C}\mathbf{u} - \mathbf{g}_0 - \mathbf{q}\mu = \mathbf{0}$$

  - Arc—length constraint

$$h(\Delta\mathbf{u}, \Delta\mu) = \frac{\Delta\mathbf{u}^T \Delta\mathbf{u}}{\psi^2} + \Delta\mu^2 - \Delta l^2 = 0$$

Numerical examples

- Compression of hexagonal honeycomb

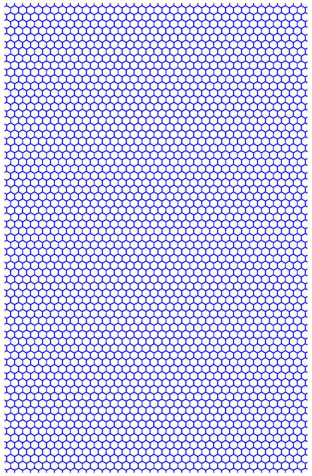


Geometry	
H	102.0 mm
L	65.8 mm
l	1.0 mm

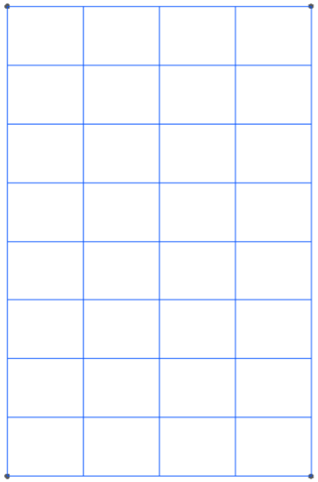
Material properties	
Bulk modulus	67.55 GPa
Shear modulus	25.90 GPa
Initial yield stress	276.0 MPa

Numerical examples

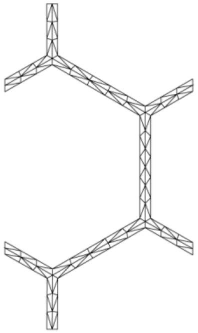
- Compression of hexagonal honeycomb: multi—scale model
  - Initiate microscopic imperfection by a random perturbation into the unit cell geometries →non—conformal mesh
  - Use second—order MCH
  - Impose second—order PBC with polynomial interpolation method



Full model



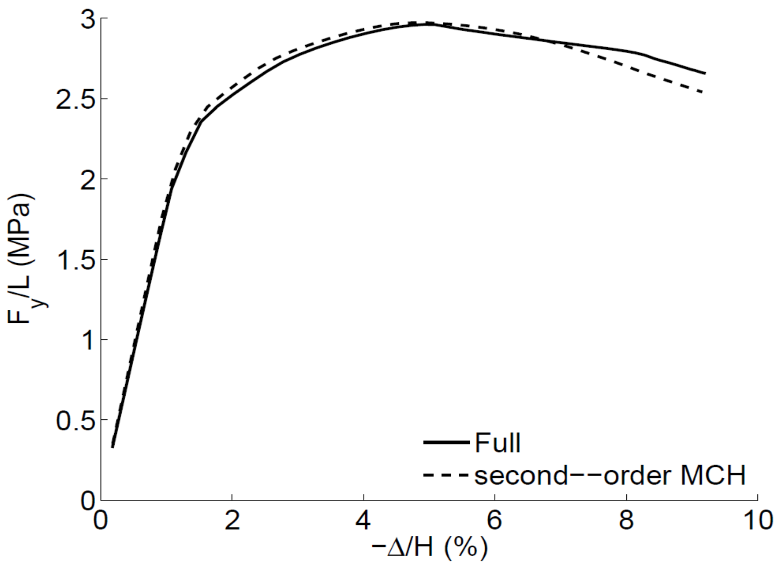
Macro—mesh



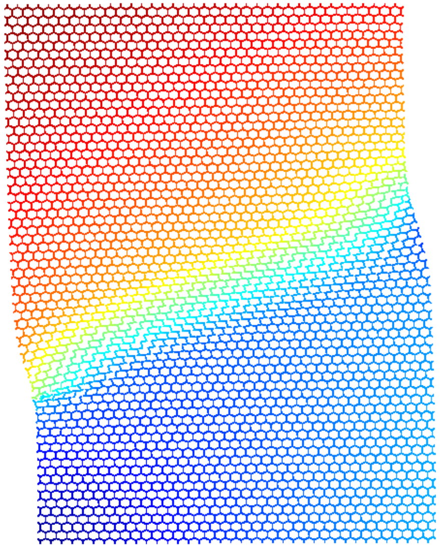
Unit cell mesh

Numerical examples

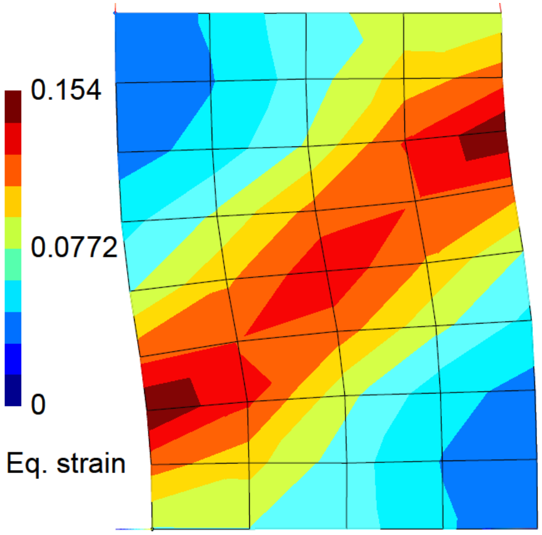
- Compression of hexagonal honeycomb: results



Action force versus prescribed displacement



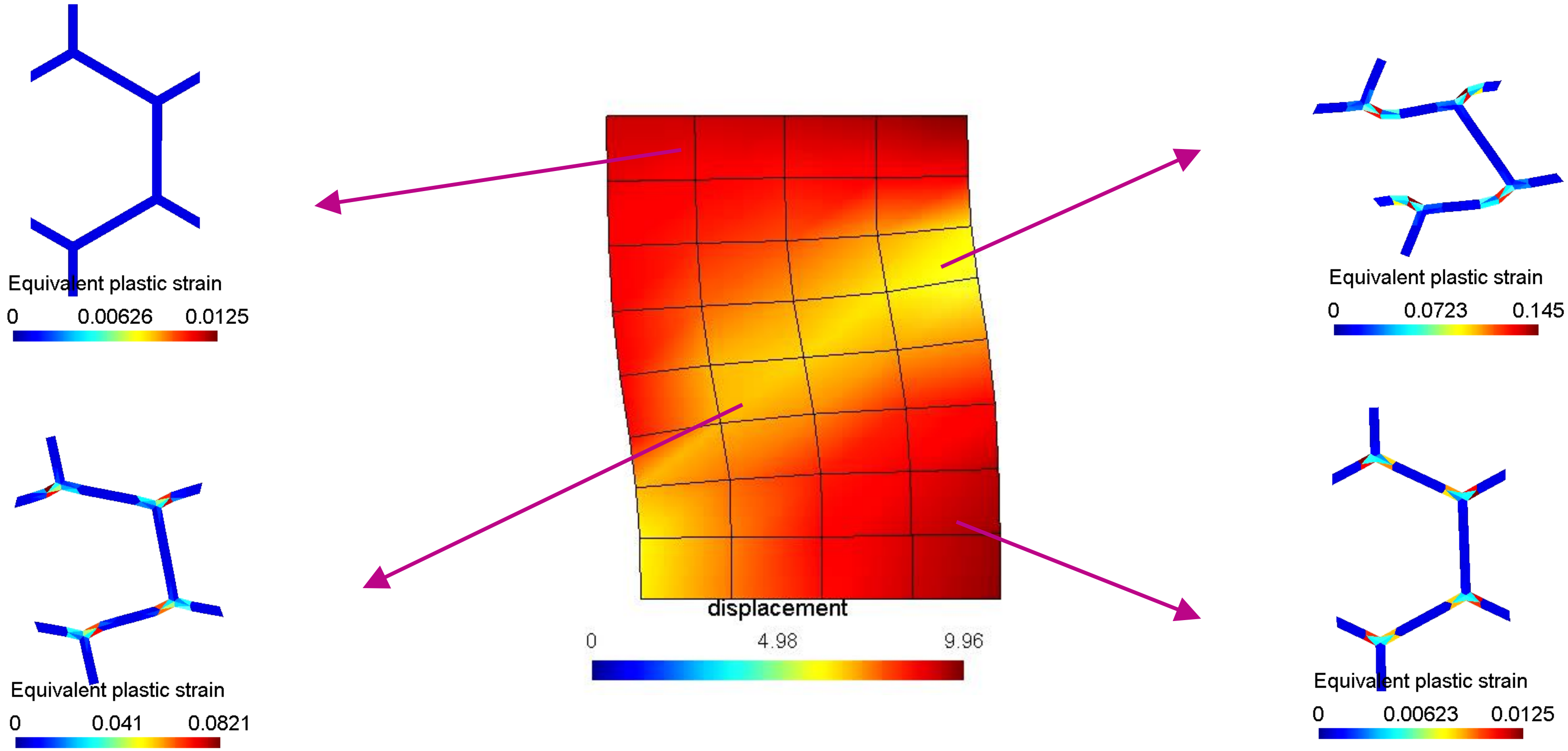
Displacement field Full model



Localization band Multi—scale model

Numerical examples

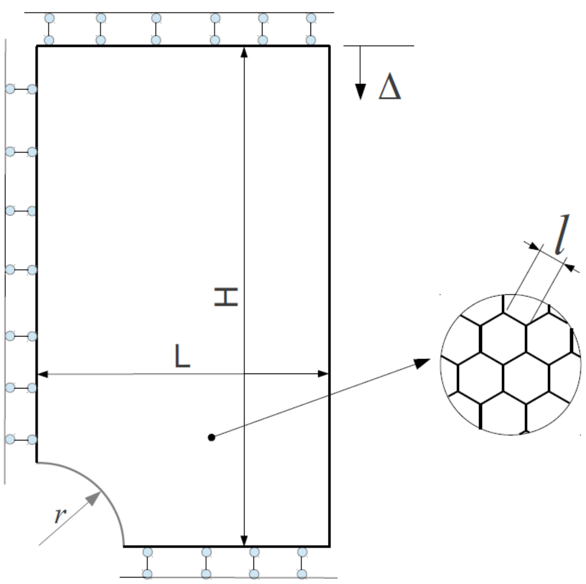
- Compression of hexagonal honeycomb: results
  - Equivalent plastic strain at several macroscopic positions



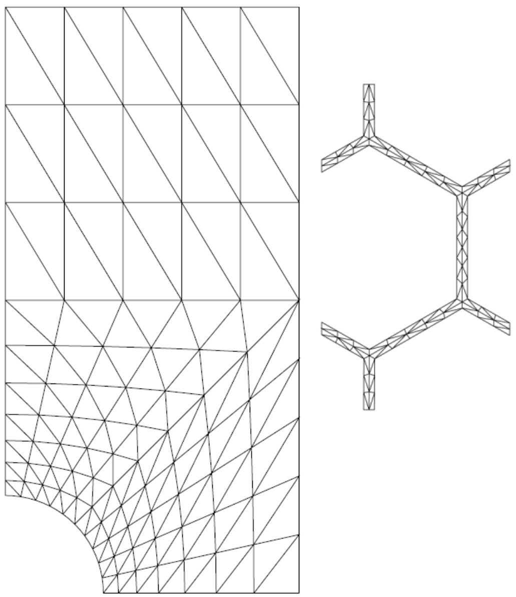
Numerical examples

- Plate with hole: size effect

Macro—Geometry	
L	3r
H	6r
l	1.0 mm

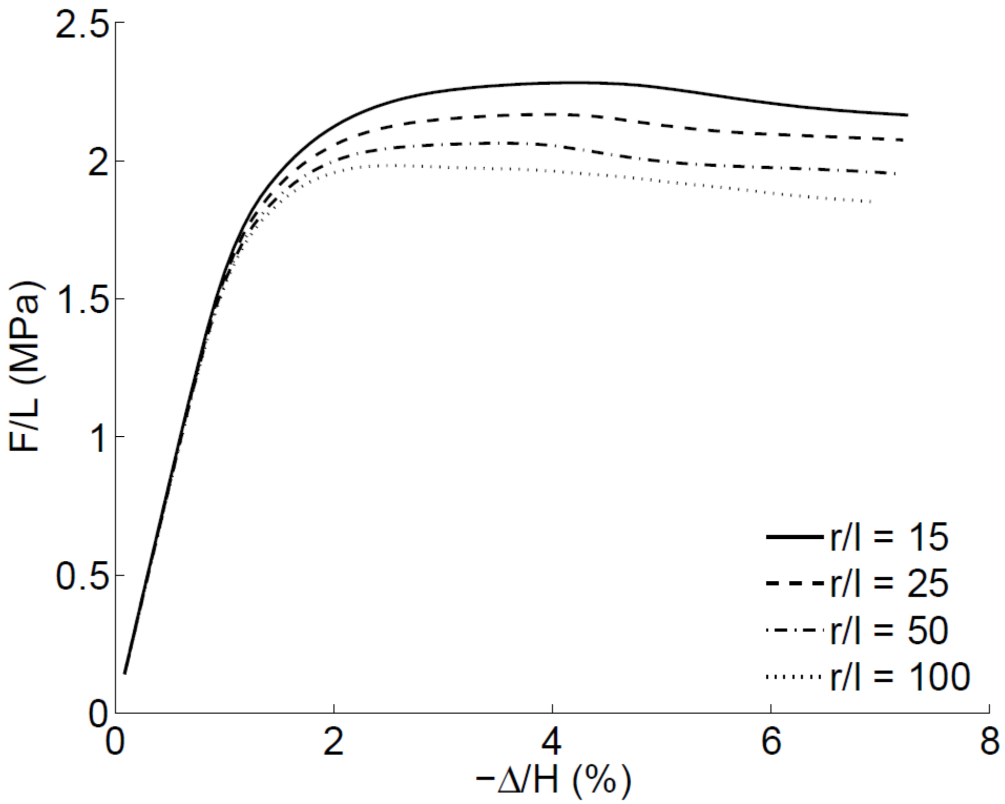


Material properties	
Bulk modulus	67.55 GPa
Shear modulus	25.90 GPa
Initial yield stress	276.0 MPa



Numerical examples

- Plate with hole: size effect results



Summary

- Using the second—order MCH to study the behavior of foamed materials
  - Moderate localization band at the macro—scale
  - Buckling at the micro—scale
  - Size effects

Thank you!