University of Liège

Department of Aerospace and Mechanical Engineering

Multi-scale computational homogenization of foams with micro-buckling

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Introduction

- Modeling of foams
  - Buckling can occur at the thin components (cell walls, cell struts), leading to
    - Macroscopic strain localization
    - Loss of the representativeness of volume elements
  - Size effects
    - Pore size

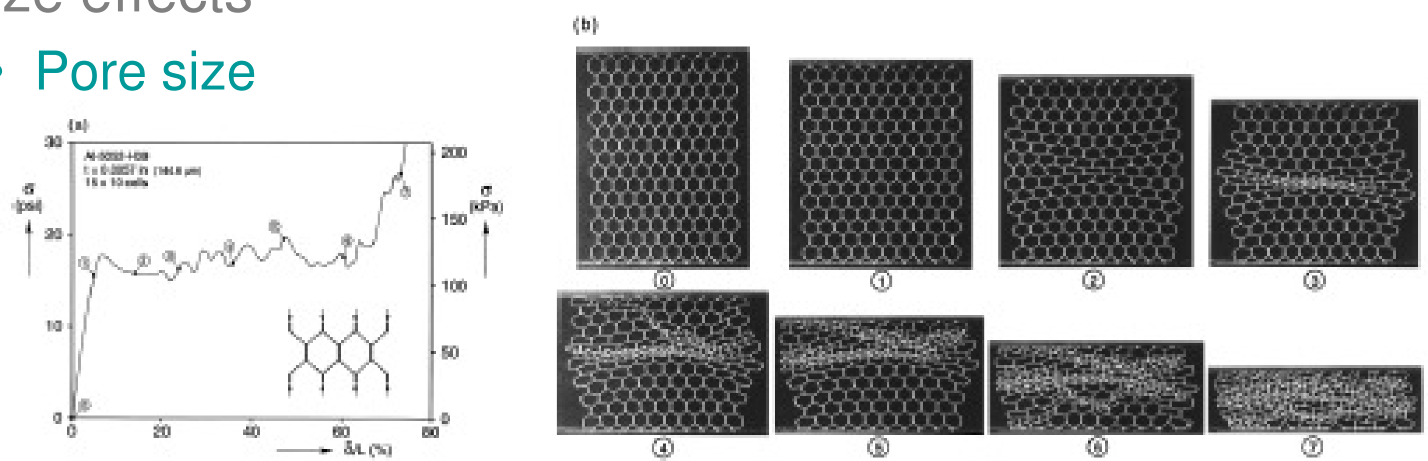
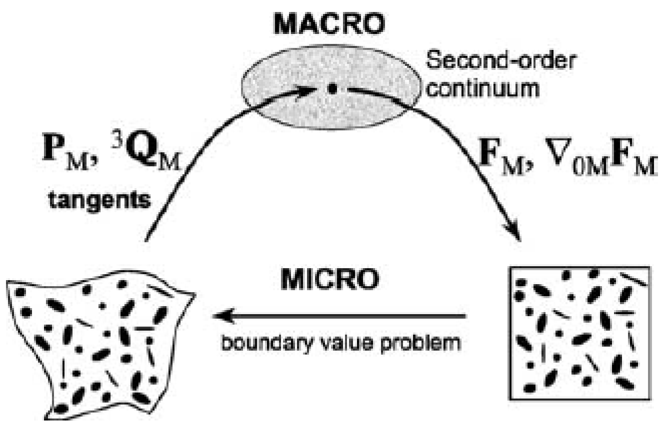


Figure: Force-displacement crushing response of polycarbonate honeycomb - S. D. Papka and S. Kyriakides (1999)

Introduction

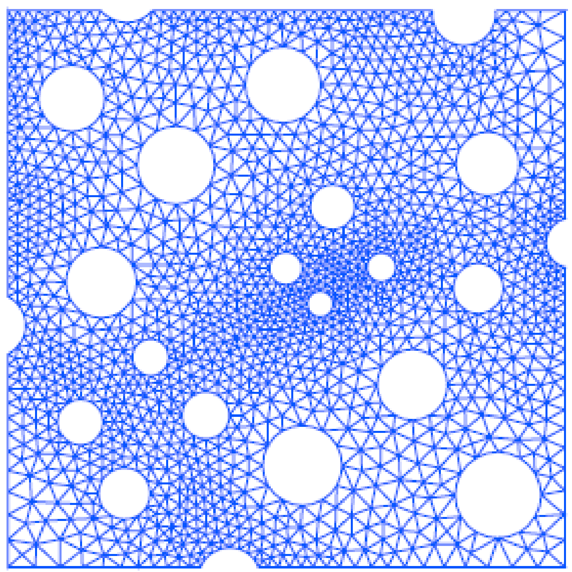
- Multi-scale computational approachs:
  - Classical multiscale computational homogenization
    - Local action → not suitable for high gradient problems and for localization analyses
    - Does not take into account the absolute size of representative volume element → not suitable for analysis of size effects
  - Second-order multiscale computational homogenization
    - Macroscopic second order continua
    - Microscopic classical continua
      - Periodic boundary condition
    - Suitable for analyses of
      - Moderate localization
      - Size effects
      - High gradient problems



Kouznetsova et al 2004

Introduction

- Modeling of foams by multi-scale computational approach
  - Using second-order multiscale computational homogenization
    - →method to solve the second-order continua
  - Using periodic boundary condition
    - Random representative volume element→non-conformal meshes
    - →method to enforce periodic boundary condition
  - Local buckling
    - Path-following

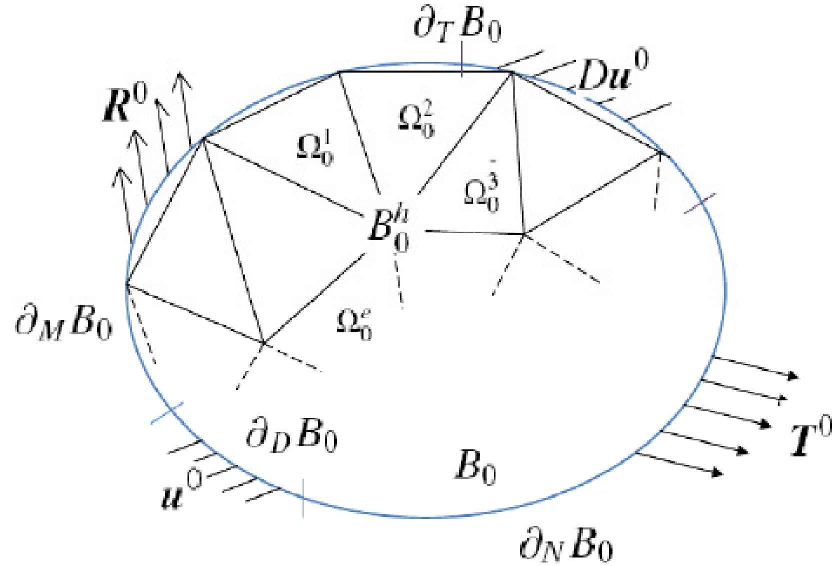


Random distributed hole structure

Introduction

- Second-order continua
  - Formulation in terms of the first Piola stress tensor **P** and second-order stress tensor **Q**

$$\boldsymbol{B} + (\boldsymbol{P} - \boldsymbol{Q} \cdot \boldsymbol{\nabla}_0) \cdot \boldsymbol{\nabla}_0 = \boldsymbol{0} \quad \forall X \in B_0$$



  - Boundary condition

$$\boldsymbol{u} = \boldsymbol{u}^0 \quad \forall X \in \partial_D B_0$$

$$D\boldsymbol{u} = D\boldsymbol{u}^0 \quad \forall X \in \partial_T B_0$$

$$(\boldsymbol{P} - \boldsymbol{Q} \cdot \boldsymbol{\nabla}_0) \cdot \boldsymbol{N} + (\boldsymbol{Q} \cdot \boldsymbol{N}) \cdot \left(\boldsymbol{N} \overset{s}{\boldsymbol{\nabla}}_0 \cdot \boldsymbol{N} - \overset{s}{\boldsymbol{\nabla}}_0\right) = \boldsymbol{T}^0 \quad \forall X \in \partial_N B_0$$

$$\boldsymbol{Q} : (\boldsymbol{N} \otimes \boldsymbol{N}) = \boldsymbol{R}^0 \quad \forall X \in \partial_M B_0$$

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Introduction

- Second-order continua
  - Requires the continuity of displacement field and of its gradients. Some methods can be considered
    - Mixed (multi-field) method (Shu et al 1999, Amanatidou et al 2002)
    - Messless method (Askes et al 2002)
    - C1 finite elements (Papanicolopulos et al 2009, 2012)
    - Discontinuous Galerkin (DG) method (Engel et al 2002, Bala Chandran et al 2008)
- In this work, DG method is extended to large deformation and multiscale analyses to solve second-order continua
  - Using only the displacement field as unknowns
  - Enforcing weakly inter-element continutities

Introduction

- Microscopic periodic boundary condition
  - Fluctuation field $\omega = u - (\bar{F} - I) \cdot X - \frac{1}{2}\bar{G} : (X \otimes X)$
  - Periodic condition of fluctuation field : (Kouznetsova et al 2004, Kaczmarczyk et al 2008)

$$\omega(X^+) = \omega(X^-) \quad \forall X^+ \in \partial V_0^+ \text{ and matching } X^- \in \partial V_0^-$$

$$\int_{S \in \partial V_0^-} \omega \, d\partial V = \mathbf{0}$$

- Finite element enforcement
  - Conformal meshes: enforcement on the matching nodes
  - For foams: non-conformal meshes:
    - Local implementation (Tyrus et al 2007)
    - Master/slave approach (Yuan et al 2008)
    - Weak periodicity (Larson et al 2011)
    - New method: polynomial interpolation (Nguyen et al 2012)

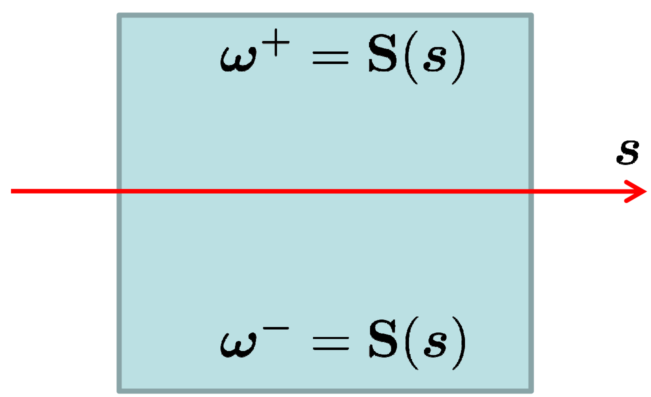
Topics

- Periodic boundary condition with foams
  - Polynomial interpolation method
- Strain-gradient continua
  - DG formulation for second-order continua
- Second-order multiscale computational homogenization with DG formulation
- Local buckling
- Conclusions and perspectives

Periodic boundary condition

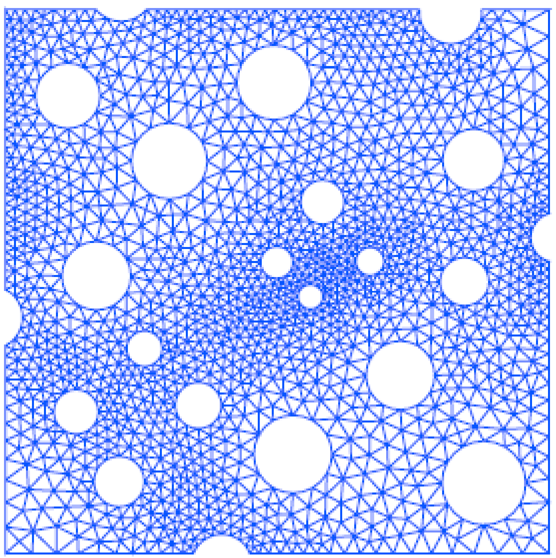
- Enforcement of periodic boundary condition in foams
  - Meshes created from foams are generally non-conformal
  - Enforcement by polynomial interpolation (Nguyen et al 2012)
    - Fluctuation field of two opposite RVE sides is interpolated by linear combinations of some shape functions
    - Degrees of freedom of two opposite RVE sides are then substituted by the coefficients of these shape functions

$$\mathbf{S}(\boldsymbol{s}) = \sum_{i=0}^{N} \mathcal{N}_i(\boldsymbol{s})\boldsymbol{a}_i$$

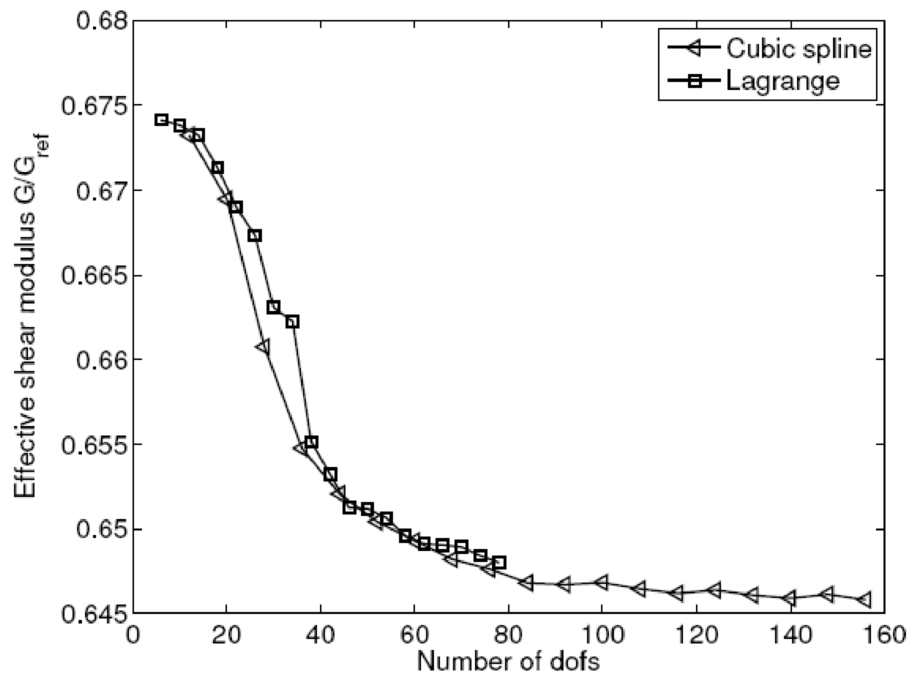


Periodic boundary condition

- Enforcement of periodic boundary condition in foams
  - Numerical example



Non-periodic mesh
from random materials



Convergence of effective property in terms of new DOFs added to the system

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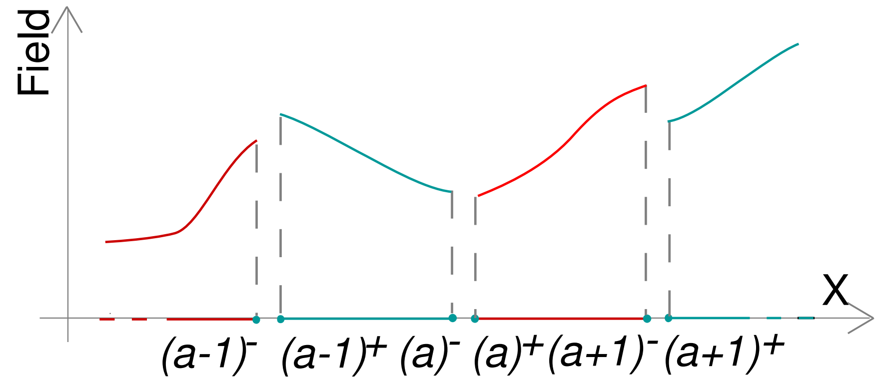
Discontinuous Galerkin formulation

- Main idea
  - Finite-element discretization
  - Same **discontinuous** polynomial approximations for the
    - **Test** functions φ_h and
    - **Trial** functions $\delta\varphi$



  - Definition of operators on the interface trace:
    - **Jump** operator: $[\![\bullet]\!] = \bullet^+ - \bullet^-$
    - **Mean** operator: $\langle\bullet\rangle = \frac{\bullet^+ + \bullet^-}{2}$
  - Continuity is weakly enforced, such that the method
    - Is consistent
    - Is stable
    - Has the optimal convergence rate

DG formulation for second-order continua

- Enriched DG formulation (EDG)
  - Strong enforcement of displacement continuity by using conventional finite element framework
  - Weak enforcement of displacement gradients by DG formulation
  - Kinematic space

$$\mathrm{U}_{\mathrm{h}}^{k} = \left\{ \boldsymbol{u}^{\boldsymbol{h}} \in \mathbf{H}^{1}\left(B_0^h\right) |_{\boldsymbol{u}^{\boldsymbol{h}}|_{\Omega_0^e} \in \mathbb{P}^k \ \ \forall \Omega_0^e \in B_0^h} \right\}$$

$$\mathrm{U}_{\mathrm{h}c}^{k} = \left\{ \delta \boldsymbol{u} \in \mathrm{U}_{\mathrm{h}}^{k} |_{\delta \boldsymbol{u}|_{\partial_D B_0} = 0} \right\}$$

- Full DG formulation (FDG)
  - Weak enforcement of displacement field and of its gradients by using DG formulation
  - Kinematic space

$$\mathrm{U}_{\mathrm{h}}^{k} = \left\{ \boldsymbol{u}^{\boldsymbol{h}} \in \mathbf{L}^{2}\left(B_0^h\right) |_{\boldsymbol{u}^{\boldsymbol{h}}|_{\Omega_0^e} \in \mathbb{P}^k \ \ \forall \Omega_0^e \in B_0^h} \right\}$$

$$\mathrm{U}_{\mathrm{h}c}^{k} = \left\{ \delta \boldsymbol{u} \in \mathrm{U}_{\mathrm{h}}^{k} |_{\delta \boldsymbol{u}|_{\partial_D B_0} = 0} \right\}$$

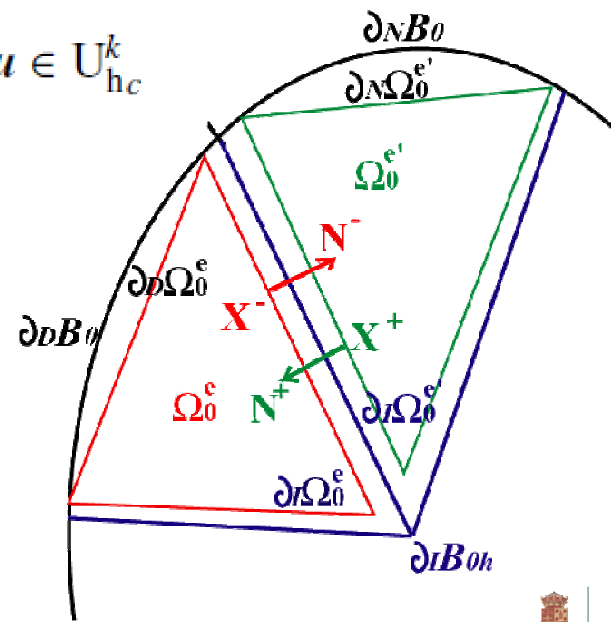
DG formulation for second-order continua

- Application to finite strain
  - Strong form:

$$\boldsymbol{B} + (\boldsymbol{P} - \boldsymbol{Q}\cdot\boldsymbol{\nabla}_0)\cdot\boldsymbol{\nabla}_0 \quad = \quad \boldsymbol{0} \quad \forall X \in B_0$$

  - Weak form: finding $\boldsymbol{u}^h \in \mathrm{U}_\mathrm{h}^k$ such that

$$\sum_e \int_{\Omega_0^e} \left\{ B_i + \frac{\partial}{\partial X_j}\left[P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k} \right] \right\} \delta u_i \, dB = 0 \qquad \forall \delta\boldsymbol{u} \in \mathrm{U}_{\mathrm{h}c}^k$$



DG formulation for second-order continua

- New weak formulation obtained by integration by parts **on each element Ω^e**

$$\sum_e \int_{\partial\Omega_0^e} N_j \left\{ \left[P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k} \right] \delta u_i + Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right\} d\partial B =$$

$$\int_{\partial B_0^h} N_j \left\{ \left[P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k} \right] \delta u_i + Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right\} d\partial B$$

$$- \int_{\partial_I B_0^h} N_j^- \left[\!\left[\hat{P}_{ij}\left(\boldsymbol{u}^h\right) \delta u_i \right]\!\right] d\partial B - \int_{\partial_I B_0^h} N_j^- \left[\!\left[Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right]\!\right] d\partial B \qquad \forall \delta\boldsymbol{u} \in \mathrm{U}_{\mathrm{h}c}^k ,$$

$$\hat{P}_{ij}\left(\boldsymbol{u}^h\right) = P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k}$$

DG formulation for second-order continua

- New weak formulation obtained by integration by parts **on each element Ω^e**

$$\sum_e \int_{\partial\Omega_0^e} N_j \left\{ \left[P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k} \right] \delta u_i + Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right\} d\partial B =$$

$$\int_{\partial B_0^h} N_j \left\{ \left[P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k} \right] \delta u_i + Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right\} d\partial B$$

$$- \int_{\partial_I B_0^h} N_j^- \left[\!\left[\hat{P}_{ij}\left(\boldsymbol{u}^h\right) \delta u_i \right]\!\right] d\partial B - \int_{\partial_I B_0^h} N_j^- \left[\!\left[Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right]\!\right] d\partial B \qquad \forall \delta\boldsymbol{u} \in \mathrm{U}_{\mathrm{hc}}^k ,$$

Interface term is neglected when using EDG

Interface terms must be considered when using EDG

$$\hat{P}_{ij}\left(\boldsymbol{u}^h\right) = P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k}$$

DG formulation for second-order continua

- New weak formulation obtained by integration by parts **on each element Ω^e**

$$\sum_e \int_{\partial\Omega_0^e} N_j \left\{ \left[P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k} \right] \delta u_i + Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right\} d\partial B =$$

$$\int_{\partial B_0^h} N_j \left\{ \left[P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k} \right] \delta u_i + Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right\} d\partial B$$

$$- \int_{\partial_I B_0^h} N_j^- \left[\!\left[\hat{P}_{ij}\left(\boldsymbol{u}^h\right) \delta u_i \right]\!\right] d\partial B - \int_{\partial_I B_0^h} N_j^- \left[\!\left[Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right]\!\right] d\partial B \qquad \forall \delta \boldsymbol{u} \in \mathrm{U}_{\mathrm{hc}}^k ,$$

Interface terms must be considered when using FDG

$$\hat{P}_{ij}\left(\boldsymbol{u}^h\right) = P_{ij}\left(\boldsymbol{u}^h\right) - \frac{\partial Q_{ijk}\left(\boldsymbol{u}^h\right)}{\partial X_k}$$

DG formulation for second-order continua

- Interface terms
  - Introduction of the numerical fluxes

$$\int_{\partial_I B_0^h} N_j^- \left[\!\left[\hat{P}_{ij}\left(\boldsymbol{u}^h\right) \delta u_i \right]\!\right] d\partial B \simeq \int_{\partial_I B_0^h} [\![\delta u_i]\!]\, h_i\left(\hat{\boldsymbol{P}}^+, \hat{\boldsymbol{P}}^-, \boldsymbol{N}^-\right) d\partial B$$

$$\int_{\partial_I B_0^h} N_j^- \left[\!\left[Q_{ijk}\left(\boldsymbol{u}^h\right) \frac{\partial \delta u_i}{\partial X_k} \right]\!\right] d\partial B \simeq \int_{\partial_I B_0^h} \left[\!\left[\frac{\partial \delta u_i}{\partial X_j} \right]\!\right] H_{ij}\left(\boldsymbol{Q}^+, \boldsymbol{Q}^-, \boldsymbol{N}^-\right) d\partial B$$

- Has to be consistent:

$$\boldsymbol{h}\left(\hat{\boldsymbol{P}}, \hat{\boldsymbol{P}}, \boldsymbol{N}\right) = \hat{\boldsymbol{P}} \cdot \boldsymbol{N} \text{ and } \boldsymbol{h}\left(\hat{\boldsymbol{P}}^+, \hat{\boldsymbol{P}}^-, \boldsymbol{N}^-\right) = -\boldsymbol{h}\left(\hat{\boldsymbol{P}}^-, \hat{\boldsymbol{P}}^+, \boldsymbol{N}^+\right)$$

$$\boldsymbol{H}\left(\boldsymbol{Q}, \boldsymbol{Q}, \boldsymbol{N}\right) = \boldsymbol{Q} \cdot \boldsymbol{N} \text{ and } \boldsymbol{H}\left(\boldsymbol{Q}^+, \boldsymbol{Q}^-, \boldsymbol{N}^-\right) = -\boldsymbol{H}\left(\boldsymbol{Q}^-, \boldsymbol{Q}^+, \boldsymbol{N}^+\right)$$

- One possible choice

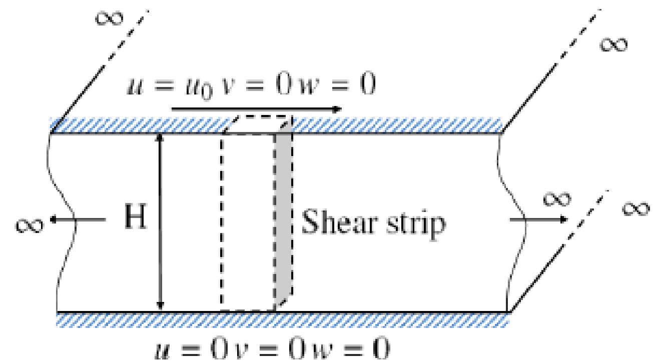
$$h_i\left(\hat{\boldsymbol{P}}^+, \hat{\boldsymbol{P}}^-, \boldsymbol{N}^-\right) = \left\langle \hat{P}_{ij} \right\rangle N_j^- + \frac{1}{2} N_j^- \left\langle \frac{\beta^P}{h^s} C^0_{ijkl} \right\rangle [\![u_k]\!]\, N_l^-$$

$$H_{ij}\left(\boldsymbol{Q}^+, \boldsymbol{Q}^-, \boldsymbol{N}^-\right) = \left\langle Q_{ijk} \right\rangle N_k^- + \frac{1}{2} N_k^- \left\langle \frac{\beta^Q}{h^s} \mathcal{J}^0_{ijkpqr} \right\rangle \left[\!\left[\frac{\partial u_p}{\partial X_q} \right]\!\right] N_r^-$$

- Stabilization controlled by parameter β, for all mesh sizes h^s

DG formulation for second-order continua

- Shear layer test: boundary effect
  - Displacement field $u = u(y)$



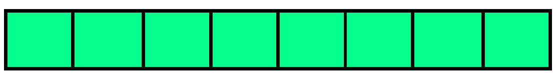
$$\frac{\partial}{\partial y}\left[\mu\frac{\partial u}{\partial y} - \frac{\partial}{\partial y}\left(\kappa\frac{\partial^2 u}{\partial y^2}\right)\right] = 0$$

$$u(0) = 0,\ \frac{\partial u}{\partial y}(0) = 0$$

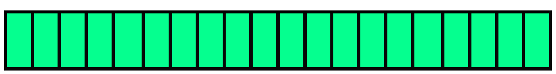
$$u(H) = u_0,\ \frac{\partial u}{\partial y}(H) = 0$$

  - Results by using FDG

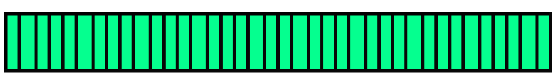
Mesh 1 (8 Elements)

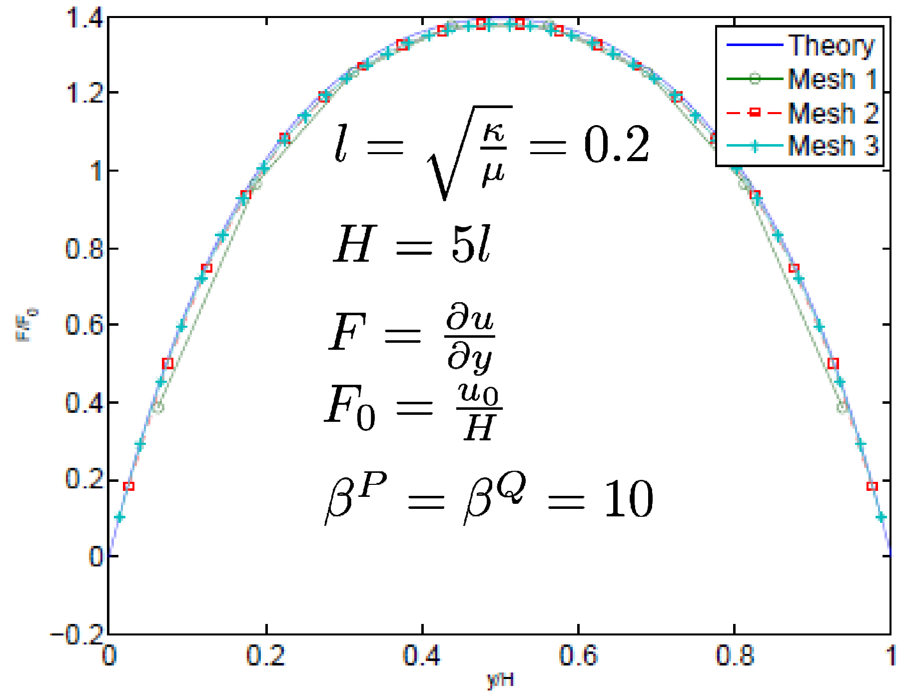


Mesh 2 (20 Elements)



Mesh 3 (38 Elements)





Multiscale scheme

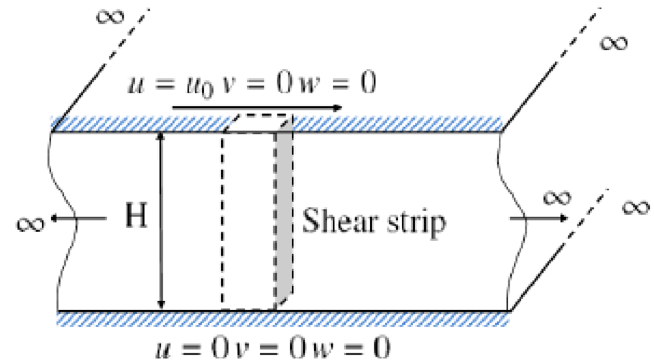
- Second-order multiscale computational homogenization with DG formulation
  - Using FDG or EDG at the macroscopic scale
  - Using conventional C^0 finite element framework at microscopic scale
  - RVEs are assigned into both surface and volume integration points
  - All microscopic boundary condition types are possible (linear displacement BC, constant traction BC, periodic BC)

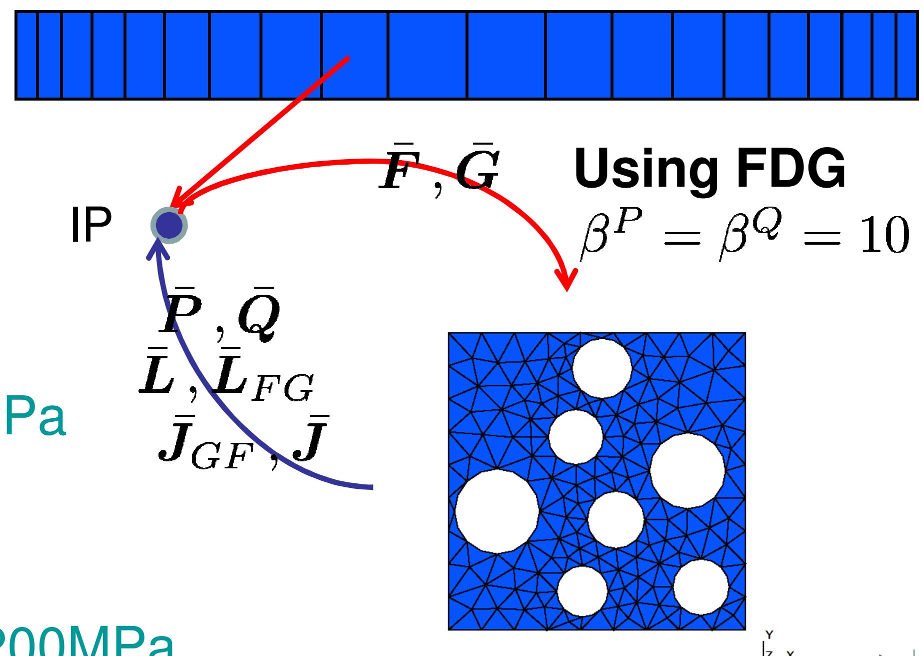
Multiscale scheme

- Shear layer problem: size effects
  - Macroscopic problem:
    - H = 1cm , 2cm, 4cm and 8cm
    - Boundary condition

$$u(0) = 0, \frac{\partial u}{\partial y}(0) = 0$$
$$u(H) = 0.01H, \frac{\partial u}{\partial y}(H) = 0$$

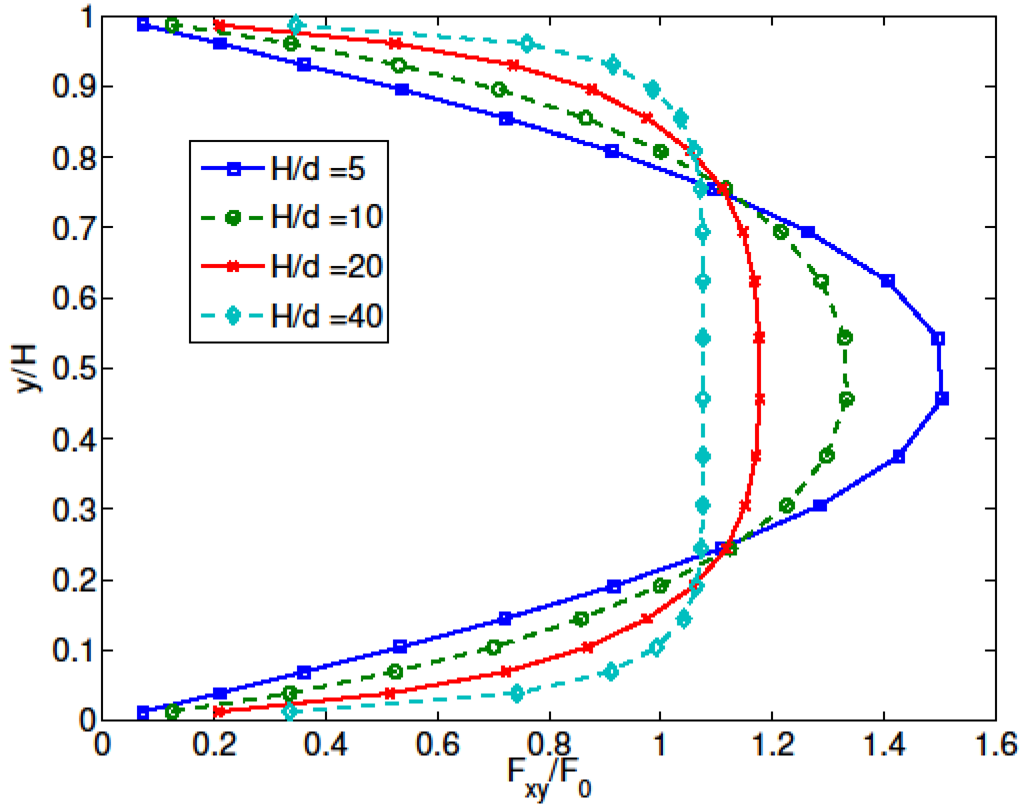
  - Microscopic problem:
    - RVE size d = 0.2cm
    - Periodic BC
    - Material law
      - Young modulus= 210GPa
      - Poisson ration= 0.3
      - Yield stress = 507MPa
      - Hardening modulus = 200MPa





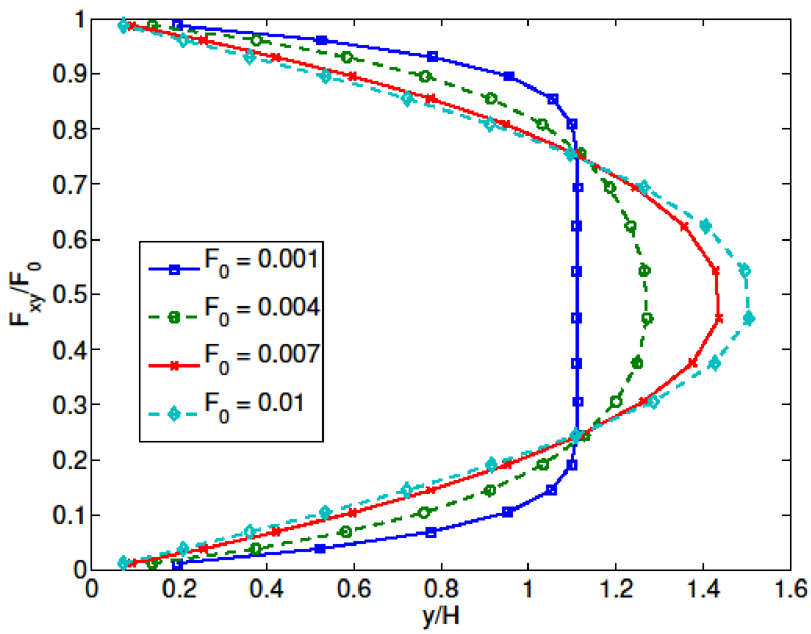
Multiscale scheme

- Shear layer problem: size effects
  - Profil of deformation gradient

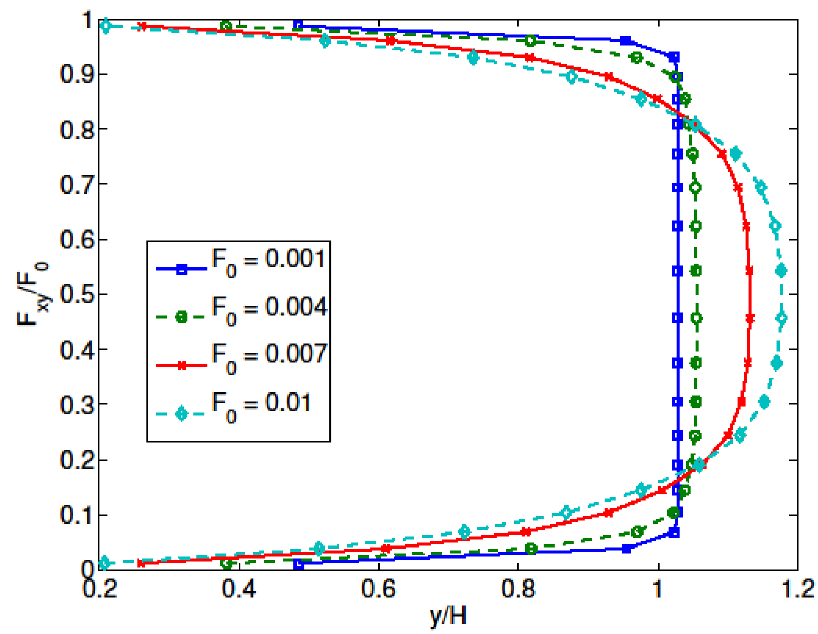


Multiscale scheme

- Shear layer problem: size effects
  - Development of boundary layer due to elastoplasticity



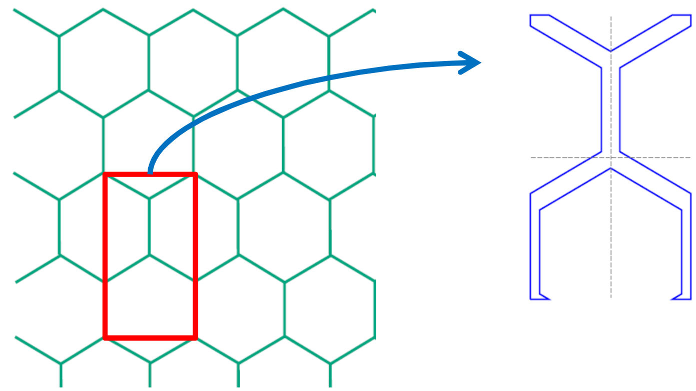
H= 1cm

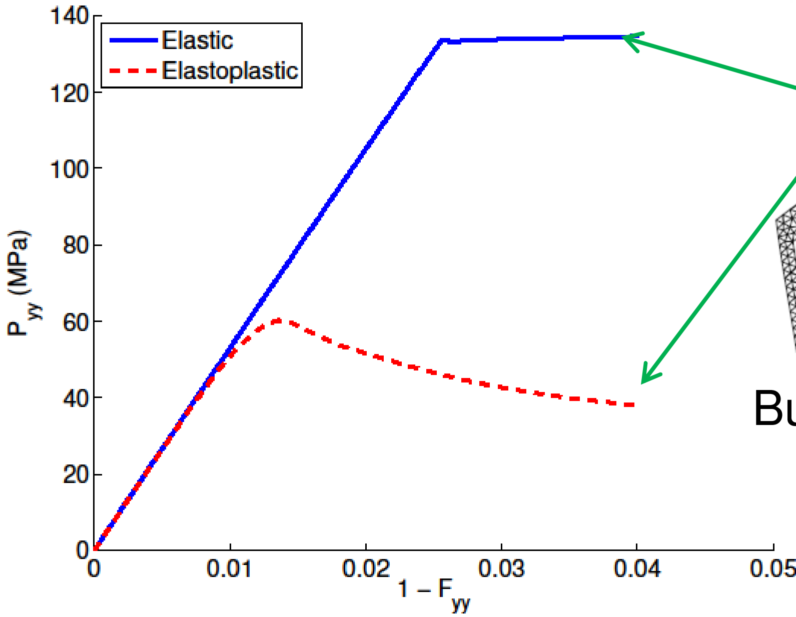


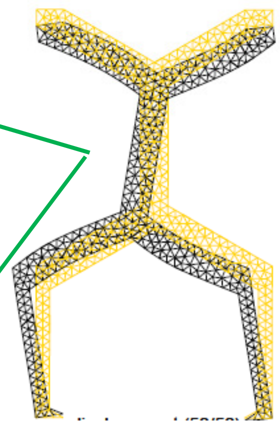
H = 4cm

Micro-buckling

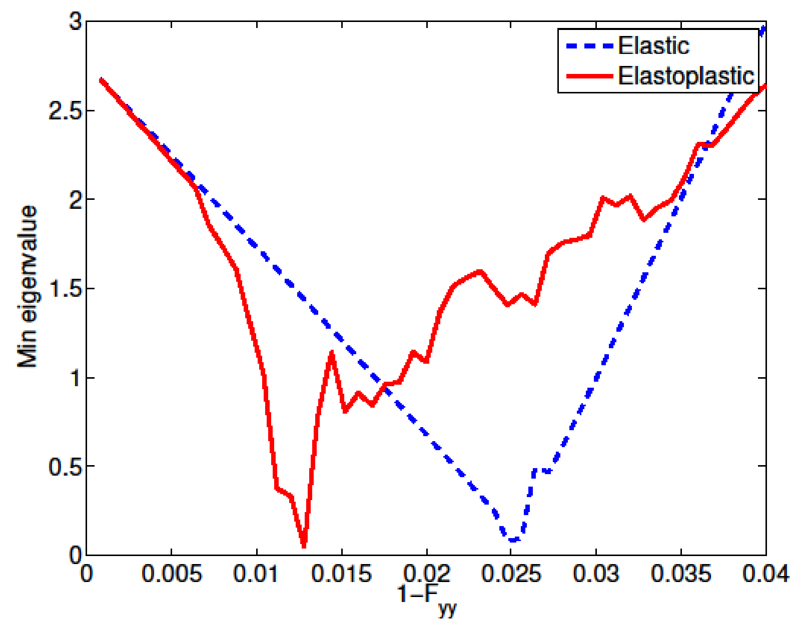
- Micro-buckling with honey-comb
  - Elastic
  - Elastoplastic







Buckling shape



Conclusions and perspectives

- Second-order computational homogenization for analyses of
  - Moderate localization
  - Size effect
  - High gradient
  - New efficient method based on DG enforcement
- Periodic boundary condition for non conforming meshes
  - Enforced by polynomial interpolation
- Analyses of local buckling
  - Based on path-following method
- Work in progress
  - Multiscale computational homogenization with micro-buckling

Thanks for your attention!