Computational homogenization of cellular materials
capturing micro-buckling, macro-localization and size effects

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Introduction

• **Cellular materials**: “a cellular solid is one made up of an interconnected network of solid struts or plates which form the edges and faces of cells”

  (Gibson & Ashby 1999)

• **Classification based on the topology**
  – Honeycombs: 2-dimensional arrays of polygons (e.g. Bee hexagons)
  – Foams: 3-dimensional network of cell edges and cell faces
    • Network of cell edges → open-cell foams
    • Network of cell faces → closed-cell foams
    • Partly open- & partly closed-cell foams

• **Man-made cellular materials**

  - Aluminum honeycomb
  - Open-cell nickel foam
  - Closed-cell polyurethane foam
Introduction

- Natural cellular materials

  (a) cork
  (b) balsa
  (c) sponge
  (d) trabecular bone
  (e) coral
  (f) cuttlefish bone
  (g) iris leaf
  (h) plant stalk

(Gibson & Ashby 1999)
Introduction

- Cellular materials are used in many applications
  - Light weight structures
  - Energy absorption
  - Packaging
  - Sound absorption
  - Thermal insulation
  - Etc.
Introduction

• ARC (Action de Recherche concertée) project

“From imaging to geometrical modeling of complex micro-structured materials: Bridging computational engineering and material science”

Material science

Computational modeling of micro-structured materials

Material tailoring

Computational engineering

Foam preparation

Tomographical images

Finite element model

Optimization analysis

Homogenized mechanical & electromagnetic properties

Converged?

Required material

An optimization procedure for “material tailoring”
Introduction

• Mechanical behavior of cellular materials
  – Buckling of thin components (cell struts, cell faces) can occur under compression loads leading to macroscopic localization

Force-displacement crushing response of aluminum honeycomb
(Experimental data from Papka & Kyriakides 1999)
Introduction

• Mechanical behavior of cellular materials (2)
  – Size effect

Effect of shear layer thickness in shear stress-strain response of Alporas foam (Experimental data from Chen & Fleck 2002)
Introduction

- Mechanical behavior of cellular materials (3)
  - Multi-scale behavior in nature
  - Intrinsic roles of different scale properties have to be accounted for
  - Macro-localization, micro-buckling, size effect phenomena have to be evaluated

Two-scale problems

(a) macroscopic continuum

(b) micro-structure with cell walls

(c) detail of cell walls with grain boundaries, other phases, inclusions, voids, etc
Introduction

• Finite element modeling strategies for cellular materials
  – Direct modeling-based approach
    • Direct models of cell struts, cell faces with beam, shell, bulk elements
  – Constitutive modeling-based approach
    • Cellular solids are considered as homogeneous media with suitable constitutive laws:
      – Phenomenological models
        » Curve fitting, parameters identification from numerical or experimental results
      – Homogenization models
        » Mean field, FFT, asymptotic, computational, etc.
Introduction

• Finite element modeling strategies for cellular materials (2)
  – Direct modeling-based approach
    • Advantages:
      – Capture directly localization due to micro-buckling & size effects

• Drawbacks
  – Enormous number of DOFs
  – Difficult to construct the FE model due to geometry complexities
  – Suitable for small problems with limited dimensions
Introduction

• Finite element modeling strategies for cellular materials (3)
  – Constitutive modeling-based approach
    • Advantages
      – Suitable for large problems
      – Micro-buckling, macro-localization & size effects can be captured with suitable constitutive models (e.g. computational homogenization)
    • Drawbacks
      – Phenomenological models
        » Details of the micro-structure during macro-loading cannot be observed
        » Material models and their parameters are difficult to be identified
      – Homogenization models
        » Occurrence of micro-buckling phenomena is still limited in the mean-field, FFT, asymptotic homogenization frameworks
Introduction

• **Computational homogenization**
  – This method is probably the most accurate method to directly account for complex micro-structural behaviors

  – This method can model:
    • Micro-buckling of cell walls (e.g. Okumura et al. 2004, Takahashi et al. 2010)
    • Localization problems (e.g. Kouznetsova et al. 2004, Massart et al. 2007, Nguyen et al. 2011, Coenen et al. 2012)
    • Size effects (e.g. Kouznetsova et al. 2004, Ebinger et al. (2005))
Introduction

• First-order computational homogenization framework (first-order FE²)
  – Macro-scale
    • Finite element model
    • At one integration point $\bar{F}$ is known, $\bar{P}$ is sought
  – Micro-scale
    • Representative Volume Element (RVE)
    • Usual finite elements
    • Microscopic boundary conditions
  – Transition
    • Down-scaling: $\bar{F}$ is used to define the BCs
    • Up-scaling: $\bar{P}$ and $\partial \bar{P}/\partial \bar{F}$ are known from resolutions of micro-scale problems
  – Scale separation

$$l_{\text{discrete}} \ll l_{\text{micro}} \ll l_{\text{macro}}$$
Introduction

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

A generalized continuum is required at the macro-scale
  – Second-order computational homogenization framework (second-order FE²) (Kouznetsova et al. 2004)
    • Macroscopic Mindlin strain gradient continuum
    • Microscopic classical continuum
    • Suitable for moderate localization bands & size effects

The numerical results change with the size of mesh and direction of mesh
The numerical results change without convergence
Introduction

- **Second-order computational homogenization framework (second-order FE²)**
  - **Macro-scale**
    - Mindlin strain gradient continuum
      \[ \mathbf{P} \otimes \nabla_0 - \mathbf{Q} : (\nabla_0 \otimes \nabla_0) = 0 \text{ in } B_0 \]
      \[ \begin{align*}
        \mathbf{\bar{u}} &= \mathbf{\bar{u}}^0 \quad \text{on } \partial_D B_0 \\
        \mathbf{\bar{T}} &= \mathbf{\bar{T}}^0 \quad \text{on } \partial_N B_0 \\
        \mathbf{D\bar{u}} &= \mathbf{D\bar{u}}^0 \quad \text{on } \partial_T B_0 \\
        \mathbf{\bar{R}} &= \mathbf{\bar{R}}^0 \quad \text{on } \partial_M B_0
      \end{align*} \]
  - **Micro-scale**
    - Usual finite elements
    - Second-order microscopic boundary conditions
  - **Transition**
    - Down-scaling: \( \mathbf{\bar{F}}, \mathbf{\bar{F}} \otimes \nabla_0 \) are used to define the BCs
    - Up-scaling: Two stresses \( \mathbf{\bar{P}}, \mathbf{\bar{Q}} \) and 4 tangent operators are known from resolutions of micro-scale problems
Introduction

• **Selected approach & challenges**
  – Microscopic classical continuum with periodic boundary condition (PBC)

→ new method to enforce PBC on non-conforming meshes
Introduction

• Selected approach & challenges (2)
  – Macroscopic Mindlin strain gradient continuum

\[ \bar{P} \otimes \nabla_0 - \bar{Q} : (\nabla_0 \otimes \nabla_0) = 0 \text{ in } B_0 \]
\&
\[ \begin{cases} \tilde{u} = \tilde{u}^0 \quad \text{on } \partial_D B_0 \\ \tilde{T} = \tilde{T}^0 \quad \text{on } \partial_N B_0 \\ D\tilde{u} = D\tilde{u}^0 \quad \text{on } \partial_T B_0 \\ \tilde{R} = \tilde{R}^0 \quad \text{on } \partial_M B_0 \end{cases} \]

⇒ efficient method to solve using usual finite elements
Introduction

• Selected approach & challenges (3)
  – Instabilities at both scales

Force-displacement crushing response of aluminum honeycomb
(Experimental data from Papka & Kyriakides 1999)

→ arc-length method to capture instabilities
Topics

- PBC enforcement based on the \textit{polynomial interpolation method}

  (Nguyen, Geuzaine, Béchet & NoelsCMS 2012)

- Second-order multi-scale computational homogenization scheme based on the Discontinuous Galerkin method (called \textit{second-order DG-based FE$^2$ scheme})
  - DG method is used to solve the macroscopic Mindlin strain gradient
  - Usual FE
  - Parallel computation

  (Nguyen, Becker & NoelsCMAME 2013)

- Use of this \textit{second-order DG-based FE$^2$ scheme} to capture instabilities in cellular materials
  - Arc-length path following method is adopted at both scales because of the presence of the macroscopic localization and micro-buckling
  - Parallel computation

  (Nguyen & NoelsIJSS 2014)
Topics

• PBC enforcement based on the *polynomial interpolation method*
  
  (Nguyen, Geuzaine, Béchet & Noels CMS 2012)

• Second-order multi-scale computational homogenization scheme based on the Discontinuous Galerkin method (called *second-order DG-based FE\(^2\) scheme*)
  
  – DG method is used to solved the macroscopic Mindlin strain gradient
  
  – Usual FE
  
  – Parallel computation

  (Nguyen, Becker & Noels CMAME 2013)

• Use of this *second DG-based FE\(^2\) scheme* to capture instabilities in cellular materials
  
  – Arc-length path following method is adopted at both scales because of the presence of the macroscopic localization and micro-buckling
  
  – Parallel computation

  (Nguyen & Noels IJSS 2014)
Polynomial interpolation method

- Periodic boundary condition
  - Defined from the fluctuation field
    - First-order: \( \mathbf{w} = \mathbf{u} - (\mathbf{F} - \mathbf{I}) \cdot \mathbf{X} \)
    - Second-order:
      \[
      \mathbf{w} = \mathbf{u} - (\mathbf{F} - \mathbf{I}) \cdot \mathbf{X} - \frac{1}{2} (\mathbf{F} \otimes \nabla_0) : (\mathbf{X} \otimes \mathbf{X})
      \]
  - Stated on the RVE boundary
    - First-order PBC:
      \[
      \mathbf{w}(\mathbf{X}^+) = \mathbf{w}(\mathbf{X}^-) \quad \text{and} \quad \mathbf{w}(\mathbf{X}^J) = \mathbf{0}
      \]
    - Second-order PBC:
      \[
      \mathbf{w}(\mathbf{X}^+) = \mathbf{w}(\mathbf{X}^-) \quad \text{and} \quad \int_{S_i} \mathbf{w}(\mathbf{X}) \, d\mathbf{V} = 0 \quad \forall S_i \subset \partial V_0
      \]
  - Can be achieved by constraining opposite nodes
Polynomial interpolation method

- **Cellular materials**
  - Usually random meshes
  - Important voids on the boundaries

- **Enforcement of the periodic boundary condition in FEM**
  - For conforming meshes
    - Directly constrains on matching nodes
  - For general meshes
    - Slave/master approach (Yuan et al. 2008)
    - Weak periodicity (Larson et al. 2011)
    - Local implementation (Tyrus et al. 2008)
    - Polynomial interpolation method (Nguyen et al. 2012)
      - For arbitrary RVE geometries

No void part on the RVE boundary
Polynomial interpolation method

- Polynomial interpolation method for PBC enforcement

  - Use of control nodes (new or existing nodes) to interpolate the fluctuation field at the RVE boundary

  - Use of interpolant functions (e.g. Lagrange, cubic spline, patch Coons, etc.)

  - Fluctuations at boundary nodes are interpolated from control nodes

  - PBC is satisfied by using the same interpolation form for opposite parts
Polynomial interpolation method

• Polynomial interpolation method for PBC enforcement (2)
  
  – First-order PBC

  \[ w^- (X) = \sum_k N^k (X) w^k + \sum_k M^k (X) \theta^k, \]

  \[ w^+ (X) = \sum_k N^k (X) w^k + \sum_k M^k (X) \theta^k \text{ and} \]

  \[ w (X^I) = 0 \]

  – Second-order PBC

  \[ w^- (X) = \sum_k N^k (X) w^k + \sum_k M^k (X) \theta^k, \]

  \[ w^+ (X) = \sum_k N^k (X) w^k + \sum_k M^k (X) \theta^k \text{ and} \]

  \[ \int_{S \subset \partial V^-} \left( \sum_k N^k (X) w^k + \sum_k M^k (X) \theta^k \right) d\partial V = 0 \]

  – Interpolant functions \( N^k, M^k \) and control DOFs \( w^k, \theta^k \) depend on the interpolation methods
Polynomial interpolation method

- Polynomial interpolation method for PBC enforcement (3)
  - Results in new constraints in terms of displacements of both boundary and control nodes
    \[ \tilde{C}\tilde{u}_b - g = 0 \]
    - First order: \( g = g(\tilde{F}) \)
    - Second-order: \( g = g(\tilde{F}, \tilde{F} \otimes \nabla_0) \)
  - These linear constraints can be enforced by
    - Constraints elimination
    - Lagrange multipliers
  - Suitable for
    - Arbitrary meshes
    - Important void parts on the RVE boundaries
    - Arbitrary interpolation forms
Polynomial interpolation method

- 2D problems using Lagrange & cubic spline interpolations
  - Periodic hole structures
    - Hole radius = 0.2 mm
    - Elastic material: Young modulus = 70 GPa, Poisson ratio = 0.3

Periodic mesh

Non-periodic mesh

Convergence of effective properties in terms of new DOFs added to system

CEM: method based on matching nodes
Polynomial interpolation method

- 2D problems using Lagrange & cubic spline interpolations (2)
  - Honeycomb structures
    - Edge length = 1 mm & thickness = 0.1 mm
    - Elastic material: Young modulus= 68.9 GPa, Poisson ratio = 0.33

RVE mesh from honeycomb structure

Convergence of effective properties in terms of new DOFs added to system
Polynomial interpolation method

- 3D problems using the patch Coons interpolation based on the Lagrange & cubic spline interpolations

\[ \bar{\varepsilon} = \begin{bmatrix} 0.01 & 0.005 & 0.005 \\ 0.005 & 0.01 & -0.005 \\ 0.005 & -0.005 & -0.01 \end{bmatrix} \]

\[ \bar{\sigma}_{\text{Lagrange}} = \begin{bmatrix} 281.583 & 92.392 & 121.181 \\ 92.392 & 270.111 & -115.835 \\ 121.181 & -115.835 & -247.78 \end{bmatrix} \text{ MPa} \]

\[ \bar{\sigma}_{\text{spline}} = \begin{bmatrix} 281.399 & 91.9833 & 121.239 \\ 91.983 & 268.85 & -115.614 \\ 121.239 & -115.614 & -248.214 \end{bmatrix} \text{ MPa} \]

Lagrange Coons patch of order 15
Cubic spline Coons patch with 10 segments
Conclusions

- A new method to enforce the PBC is presented
  - By using an interpolation formulation
  - For arbitrary meshes
  - For both 2-dimensional and 3-dimensional problems

- This method provides a better estimation compared to the linear displacement BC which is usually used for non-conforming meshes

- The key advantage of this method is the elimination of the need of matching nodes
Topics

• PBC enforcement based on the *polynomial interpolation method*  
  (Nguyen, Geuzaine, Béchet & Noels  CMS 2012)

• **Second-order multi-scale computational homogenization scheme based on the Discontinuous Galerkin method (called second-order DG-based FE\(^2\) scheme)**
  
  – DG method is used to solved the macroscopic Mindlin strain gradient
  
  – Usual FE
  
  – Parallel computation
  
  (Nguyen, Becker & Noels  CMAME 2013)

• Use of this second DG-based FE\(^2\) scheme to capture instabilities in cellular materials
  
  – Arc-length path following method is adopted at both scales because of the presence of the macroscopic localization and micro-buckling
  
  – Parallel computation
  
  (Nguyen & Noels  IJSS 2014)
Mindlin strain gradient problem

• Mindlin strain gradient

\[ \bar{P} \otimes \nabla_0 - \bar{Q} : (\nabla_0 \otimes \nabla_0) = 0 \quad \text{in } B_0 \quad \& \quad \begin{cases} \bar{u} = \bar{u}^0 & \text{on } \partial_D B_0 \\ \bar{T} = \bar{T}^0 & \text{on } \partial_N B_0 \\ D\bar{u} = D\bar{u}^0 & \text{on } \partial_T B_0 \\ \bar{R} = \bar{R}^0 & \text{on } \partial_M B_0 \end{cases} \]

• Numerical solution requires the continuity of the displacement field and of its derivatives. Some methods can be considered:
  – Mixed methods (e.g. Shu et al. 1999)
  – Mesh-less method (e.g. Askes et al. 2002)
  – \( C^1 \) finite elements (e.g. Papanicolopulos et al. 2012)
  – Discontinuous Galerkin (DG) method (e.g. Engel et al. 2002)

• DG method is extended to large deformations and multi-scale analyses to solve the Mindlin strain gradient continuum
  – Using only the displacement field as unknowns
  – Enforcing weakly inter-element continuities
Key principles of DG method

- Finite element discretization
- Same **discontinuous** polynomial approximation for
  - Test function $\varphi_h$
  - Trial function $\delta \varphi$

- Definition of trace operators on the inter-element interfaces
  - Jump operator $[\bullet] = \bullet^+ - \bullet^-$
  - Mean operator $\langle \bullet \rangle = \frac{1}{2} (\bullet^+ + \bullet^-)$

- Continuity is weakly enforced, such that the method
  - Is consistent
  - Is stable
  - Has an optimal convergence rate
DG method for strain gradient problems

- As the strain gradient solution requires the $C^0$ & $C^1$ continuities, two formulations can be used:
  - Full Discontinuous Galerkin (FDG) formulation
    \[
    \begin{align*}
    \mathbf{U}^k &= \left\{ \mathbf{u} \in L^2(B_0) \mid \mathbf{u}|_{\Omega_0} \in P^k \forall \Omega_0 \in B_0 \right\} \\
    \mathbf{U}_c^k &= \left\{ \delta \mathbf{u} \in \mathbf{U}^k \mid \delta \mathbf{u}|_{\partial DB_0} = 0 \right\}
    \end{align*}
    \]
    - Weak enforcement of $C^0$ & $C^1$ continuities
    - Different DOFs at inter-element interfaces
    - Usual shape functions
  - Enriched Discontinuous Galerkin (EDG) formulation
    \[
    \begin{align*}
    \mathbf{U}^k &= \left\{ \mathbf{u} \in H^1(B_0) \mid \mathbf{u}|_{\Omega_0} \in P^k \forall \Omega_0 \in B_0 \right\} \\
    \mathbf{U}_c^k &= \left\{ \delta \mathbf{u} \in \mathbf{U}^k \mid \delta \mathbf{u}|_{\partial DB_0} = 0 \right\}
    \end{align*}
    \]
    - Weak enforcement of $C^1$ continuity
    - Same DOFs as conventional FEM
    - Usual shape functions
DG method for strain gradient problems

- Weak formulation obtained by repeating integrations by parts on each element:

\[ \sum_e \int_{\Omega_e^0} \delta \vec{u} \cdot [\bar{\mathbf{P}} \otimes \nabla_0 - \bar{\mathbf{Q}} : (\nabla_0 \otimes \nabla_0)] \, dB = 0 \]

\[ \int_{\partial B_0} \delta \vec{u} \cdot \bar{\mathbf{P}} \cdot \bar{\mathbf{N}} + (\delta \vec{u} \otimes \nabla_0) : (\bar{\mathbf{Q}} \cdot \bar{\mathbf{N}}) \, d\partial B \]

\[ + \sum_e \int_{\partial I \Omega_e^0} \delta \vec{u} \cdot \bar{\mathbf{P}} \cdot \bar{\mathbf{N}} + (\delta \vec{u} \otimes \nabla_0) : \bar{\mathbf{Q}} \cdot \bar{\mathbf{N}} \, d\partial B \]

\[ - \int_{B_0} \left[ \bar{\mathbf{P}} : (\delta \vec{u} \otimes \nabla_0) + \bar{\mathbf{Q}} : (\delta \vec{u} \otimes \nabla_0 \otimes \nabla_0) \right] \, dB = 0 \]

\[ \bar{\mathbf{P}} = \bar{\mathbf{P}} - \bar{\mathbf{Q}} : \nabla_0 \]
DG method for strain gradient problems

• First-order interface term

\[ \int_{\partial_I B_0} \left[ \delta \tilde{u} \cdot \tilde{P} \right] \cdot \tilde{N} \, d\partial B \]

is rewritten as the sum of three terms:

- Consistency

\[ \int_{\partial_I B_0} \left[ \delta \tilde{u} \right] \cdot \left\langle \tilde{P} \right\rangle \cdot \tilde{N}^- \, d\partial B \]

- Compatibility

\[ \int_{\partial_I B_0} \left[ \tilde{u} \right] \cdot \left\langle \tilde{P} (\delta \tilde{u}) \right\rangle \cdot \tilde{N}^- \, d\partial B \]

- Stability controlled by \( \beta_P \)

\[ \int_{\partial_I B_0} \left( [\tilde{u}] \otimes \tilde{N}^- \right) : \left\langle \frac{\beta_P}{h_s} C^0 \right\rangle : \left( \delta \tilde{u} \otimes \tilde{N}^- \right) \, d\partial B \]

These terms vanish in the case of EDG formulation

• Second-order interface term

\[ \int_{\partial_I B_0} \left[ (\delta \tilde{u} \otimes \nabla_0) : \tilde{Q} \right] \cdot \tilde{N} \, d\partial B \]

is rewritten as the sum of three terms:

- Consistency

\[ \int_{\partial_I B_0} \left[ \delta \tilde{u} \otimes \nabla_0 \right] : \left\langle \tilde{Q} \right\rangle \cdot \tilde{N}^- \, d\partial B \]

- Compatibility

\[ \int_{\partial_I B_0} \left[ \tilde{u} \otimes \nabla_0 \right] : \left\langle \tilde{Q} (\delta \tilde{u}) \right\rangle \cdot \tilde{N}^- \, d\partial B \]

- Stability controlled by \( \beta_Q \)

\[ \int_{\partial_I B_0} \left( [\tilde{u} \otimes \nabla_0] \otimes \tilde{N}^- \right) : \left\langle \frac{\beta_Q}{h_s} J^0 \right\rangle : \left( [\delta \tilde{u} \otimes \nabla_0] \otimes \tilde{N}^- \right) \, d\partial B \]

\( h_s \) characteristic mesh size
DG method for strain gradient problems

- Weak formulation obtained by DG method: \( a (\bar{u}, \delta \bar{u}) = b (\delta \bar{u}) \quad \forall \delta \bar{u} \in U^K_c \)

- Bi-nonlinear term: \( a (\bar{u}, \delta \bar{u}) = a^{\text{bulk}} (\bar{u}, \delta \bar{u}) + a^{\text{PL}} (\bar{u}, \delta \bar{u}) + a^{\text{QI}} (\bar{u}, \delta \bar{u}) \)
  - Bulk term
    \[
a^{\text{bulk}} (\bar{u}, \delta \bar{u}) = \int_{B_0} \left[ \bar{P} : (\delta \bar{u} \otimes \nabla_0) + \bar{Q} : (\delta \bar{u} \otimes \nabla_0 \otimes \nabla_0) \right] dB
    \]
  - First-order interface term (vanishes if using the EDG formulation)
    \[
a^{\text{PL}} (\bar{u}, \delta \bar{u}) = \int_{\partial_1 B_0} \left[ \| \delta \bar{u} \| \cdot \langle \bar{P} (\bar{u}) \rangle \cdot \hat{N}^- + \| \bar{u} \| \cdot \langle \bar{P} (\delta \bar{u}) \rangle \cdot \hat{N}^- \ight.
    \]
    \[
    + [\| \bar{u} \| \otimes \hat{N}^- : \left( \frac{\beta_P}{h_s} C^0 \right) : [\| \delta \bar{u} \| \otimes \hat{N}^-] \] \[ d\partial B ,
    \]
  - Second-order interface term
    \[
a^{\text{QI}} (\bar{u}, \delta \bar{u}) = \int_{\partial_1 B_0} \left[ [\delta \bar{u} \otimes \nabla_0] : \langle \bar{Q} (\bar{u}) \rangle \cdot \hat{N}^- + [\bar{u} \otimes \nabla_0] : \langle \bar{Q} (\delta \bar{u}) \rangle \cdot \hat{N}^- \ight]
    \[
    + [\| \bar{u} \| \otimes \hat{N}^- : \left( \frac{\beta_Q}{h_s} J^0 \right) : [\| \delta \bar{u} \| \otimes \nabla_0 \otimes \hat{N}^-] \] \[ d\partial B .
    \]

- Load term
  \[
b (\delta \bar{u}) = \left( \int_{\partial N B_0} \bar{T}^0 \cdot \delta \bar{u} d\partial B + \int_{\partial M B_0} \bar{R}^0 \cdot D\delta \bar{u} d\partial B \right)
  \]
DG method for strain gradient problems

- **Second-order DG-based FE² scheme**
  - DG solution of macroscopic Mindlin strain gradient problems
    - Interface & bulk integration points

- Microscopic problems
  - Associated with both interface & bulk integration points

- Scale transitions
  - Down-scaling: two kinematic strains are used to define the microscopic BCs
  - Up-scaling: two stresses and 4 tangent operators are extracted from the resolutions of the microscopic problems
DG method for strain gradient problems

• Parallel second-order DG-based FE$^2$ scheme
  – Computation strategy

Distribute to $n$ processors (macro-procs)

Distribute micro-BVPs in each partition to $p$ processors (micro-procs)

Solve the micro-problems
DG method for strain gradient problems

• Parallel second-order DG-based FE² scheme (2)
  – At the macro-scale
    • Macro-scale parallelization
    • Computation using FDG formulation with “ghost elements”
      – Communications required at each time step to exchange the nodal displacements at inter-partition interfaces only
  – At the micro-scale
    • All microscopic problems are separate in nature

(Becker et al. 2012, Wu et al. 2013)
DG method for strain gradient problems

• Multi-scale study of the shear layer test
  – $H = 1\text{cm}, 2\text{cm}, 4\text{cm}$ and $8\text{cm}$ in order to consider size effects
  – RVE size $d = 0.2\text{cm}$
  – Material law
    • Bulk modulus = 175 GPa
    • Shear modulus = 81 GPa
    • Yield stress = 507 MPa
    • Hardening modulus = 200 MPa
DG method for strain gradient problems

- Multi-scale study of the shear layer test (2)
  - Size effect

Deformation profile

Deformed shape with $H/d = 10$

Deformed shape with $H/d = 40$
DG method for strain gradient problems

• Conclusions
  – The Mindlin strain gradient problems are solved using the discontinuous Galerkin formulations with conventional finite elements
  – The resulting one-field formulation can easily be implemented in existing software
  – This formulation is used for second-order multi-scale computational homogenizations
  – The micro and macro-scale problems consider finite strains
  – Size effects in heterogeneous elasto–plastic materials can be studied
Topics

• PBC enforcement based on the polynomial interpolation method
  (Nguyen, Geuzaine, Béchet & Noels  CMS 2012)

• Second-order multi-scale computational homogenization scheme based on the Discontinuous Galerkin method (called second-order DG-based FE2 scheme)
  – DG method is used to solved the macroscopic Mindlin strain gradient
  – Usual FE
  – Parallel computation
  (Nguyen, Becker & Noels CMAME 2013)

• Use of this second-order DG-based FE$^2$ scheme to capture instabilities in cellular materials
  – Arc-length path following method is adopted at both scales because of the presence of the macroscopic localization and micro-buckling
  – Parallel computation
  (Nguyen & Noels IJSS 2014)
Second-order DG-based FE\(^2\) scheme for cellular materials

- **Microscopic classical continuum**
  - Enforcement of PBC using the polynomial interpolation method
  - Arc-length path following method

- **Macroscopic Mindlin strain gradient continuum**
  - Resolution with Discontinuous Galerkin formulation
  - Arc-length path following method

- **Full parallel computations**
  - Macroscopic parallel distribution using ghost elements
  - Microscopic parallel distribution

- **Why the arc-length path following method?**
  - Load-based increments (pure load, arc-length increments, etc.) are preferred to improve the Newton-Raphson convergence
  - Presence of critical points (e.g. limit points) & unstable equilibrium paths for which the conventional Newton-Raphson method fails → arc-length increments
Second-order DG-based FE² scheme for cellular materials

- **Path following method**
  - **Macro-scale problem**
    - Path following with applied loading
      \[
a(\tilde{\mathbf{u}}, \delta \tilde{\mathbf{u}}) = \tilde{\mu} b(\delta \tilde{\mathbf{u}})
      \]
    - Arc-length constraint
      \[
      \tilde{h}(\Delta \tilde{\mathbf{u}}, \Delta \tilde{\mu}) = \frac{\Delta \tilde{\mathbf{u}}^T \Delta \tilde{\mathbf{u}}}{\psi^2} + \Delta \tilde{\mu}^2 - \Delta l^2 = 0
      \]
  - **Micro-scale problems**
    - Path following method on the applied boundary conditions
      \[
      \tilde{\mathbf{C}}\tilde{\mathbf{u}}_b - g(\tilde{\mathbf{F}}, \tilde{\mathbf{F}} \otimes \nabla_0) = 0
      \]
      \[
      (\tilde{\mathbf{F}}, \tilde{\mathbf{F}} \otimes \nabla_0) = (\tilde{\mathbf{F}}, \tilde{\mathbf{F}} \otimes \nabla_0)_0
      + \mu [ (\tilde{\mathbf{F}}, \tilde{\mathbf{F}} \otimes \nabla_0)_{1} - (\tilde{\mathbf{F}}, \tilde{\mathbf{F}} \otimes \nabla_0)_{0} ]
      \]
    - Arc-length constraint
      \[
      h(\Delta \mathbf{u}, \Delta \mu) = \frac{\Delta \mathbf{u}^T \Delta \mathbf{u}}{\psi^2} + \Delta \mu^2 - \Delta l^2 = 0
      \]
    - Compute by increments until \( \mu = 1 \)
Second-order DG-based FE² scheme for cellular materials

- Compression of an hexagonal honeycomb plate
  - Plate: $H = 102$ mm, $L = 65.8$mm
  - Honeycomb: $l = 1$ mm, $t = 0.1$ mm
  - Elasto-plastic material
    - Bulk modulus = 67.55 GPa
    - Shear modulus = 25.9 GPa
    - Initial yield stress = 276 MPa

Full model

Mesh 0

Mesh 1

Mesh 2

Unit cell mesh
Second-order DG-based FE² scheme for cellular materials

- Compression of an hexagonal honeycomb plate (2)
  - Captures the softening onset
  - Captures the softening response
  - No macro-mesh size effect
Second-order DG-based FE$^2$ scheme for cellular materials

- Compression of an hexagonal honeycomb plate (3)
  - Influence of cell size
    - Same honeycomb structure: $l = 1$ mm, $t = 0.1$ mm
    - Different plate dimensions

(a) overall response

(b) zoom at the strain softening onset
Second-order DG-based FE² scheme for cellular materials

- Compression of a hexagonal honeycomb plate with a centered hole
  - Central radius: \( r = 15 \) mm
  - Honeycomb: \( l = 1 \) mm, \( t = 0.1 \) mm
  - Elasto-plastic material
    - Bulk modulus = 67.55 GPa
    - Shear modulus = 25.9 GPa
    - Initial yield stress = 276 MPa

Geometry & BCs

Full model with 300,000 quadratic triangles

Multi-scale model
Second-order DG-based FE\textsuperscript{2} scheme for cellular materials

- Compression of a hexagonal honeycomb plate with a centered hole (2)
  - Results given by full and multi-scale models are comparable
A second-order DG-based FE² scheme was developed with the following novelties:

- The periodic boundary condition is enforced using the polynomial interpolation method without the need of conforming meshes.

- The macroscopic Mindlin strain gradient problem is solved using the Discontinuous Galerkin method with conventional finite elements.

- The arc-length path following method is applied at both scales to capture their instabilities.
Current works

• Polypropylene foam
  – Experimental tests (F. Wan)

  ![SEM image of a PP foam with 4% CNTs](image)

  **Imperfections → reduce the stiffness**
  – Random cell sizes and shapes
  – Non-uniform distribution of solid materials of cell walls
  – Curvature of cell walls
  – Loss of cell walls
  – Corrugation of cell walls
  – Fracture of cell walls
  – ...

![Stress-strain curve](chart)
Current works

- Homogenized properties based on the tetrakaidecahedron unit cell
  - Ideal unit cell models

![Closed unit cell](image)

![Open unit cell](image)

→ Imperfections must be considered
Current works

- Homogenized properties based on the tetrakaidecahedron unit cell (2)
  - Unit cell with mass concentration at cell edges
- Mass concentration parameter: $\phi = \text{mass at cell edge/ total mass}$

![Diagram showing homogenized properties and reduced modulus graph]
Perspectives

• Experimental validation in the context of the ARC project with the RVE meshes coming from tomographical images of the microstructure

• Electromagnetic-mechanical coupling problems since electromagnetic properties are modified during the mechanical loading (as the shape is deformed)

• Discontinuous-continuous schemes for sharper localization problems following the works of Massart et al. 2007, Nguyen et al. 2011 or Coenen et al. 2012

• Material tailoring with required properties by computational homogenization schemes

• ...
Thank you for your attention!
Annex 1 - Macro-scale path following resolution

Initialization

Adjust $\Delta L$

Assemble stiffness

Predictor step

Update increment

Corrector step

End

YES

NO

$\bar{L} \geq L_{\text{max}}$

Compute macro—strains at all Gauss points

Send macro—strains to microscopic BVPs

Solve all micro--BVPs

Homogenized stresses and tangents

Assemble stiffness

Store solution and set initial state for all micro—BVPs

YES

NO

$\bar{\varepsilon} < \text{Tol}$

Compute residual
Annex 2 - Micro-scale path following resolution

Parameterize with $\mu$ and load the microscopic state reached at the end of the previous macro arc-length increment

$\mathbf{F}, \mathbf{F} \otimes \mathbf{\nabla}_0$

Adjust $\Delta l$

Compute stiffness & load vector

Predictor step

Update increment and compute strain

Corrector step

Load control

$\Delta l = 1 - \mu_{prev}$

Load control

$\mu_{prev} = \mu$

$\mu = \mu + \Delta \mu$

$\varepsilon < \text{Tol}$

Compute residual

$\mu = 1$

Extract macro—properties

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

Tangent operators

Store data for next step

Update displacement field

YES

$\mu > 1$

NO

YES

Compute stiffness & load vector

NO

YES

NO

$\mu_{prev} = \mu$

$\mu = \mu + \Delta \mu$

$\varepsilon < \text{Tol}$

Compute residual

$\mu = 1$

Extract macro—properties

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

Tangent operators

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### Annex 3 – Computation time

<table>
<thead>
<tr>
<th>Method</th>
<th>CPU time per iteration</th>
<th>Used memory</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full model</td>
<td>92 seconds</td>
<td>5.6 gigabytes</td>
</tr>
<tr>
<td>Multi–scale model, mesh 0</td>
<td>36 seconds</td>
<td>1.3 gigabytes</td>
</tr>
<tr>
<td>Multi–scale model, mesh 1</td>
<td>84 seconds</td>
<td>2.6 gigabytes</td>
</tr>
<tr>
<td>Multi–scale model, mesh 2</td>
<td>146 seconds</td>
<td>4.0 gigabytes</td>
</tr>
</tbody>
</table>

Computation time and used memory of the full model and multi–scale models. These computations were performed in the same machine with one processor.