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Imposing periodic boundary condition on arbitrary meshes by polynomial interpolation

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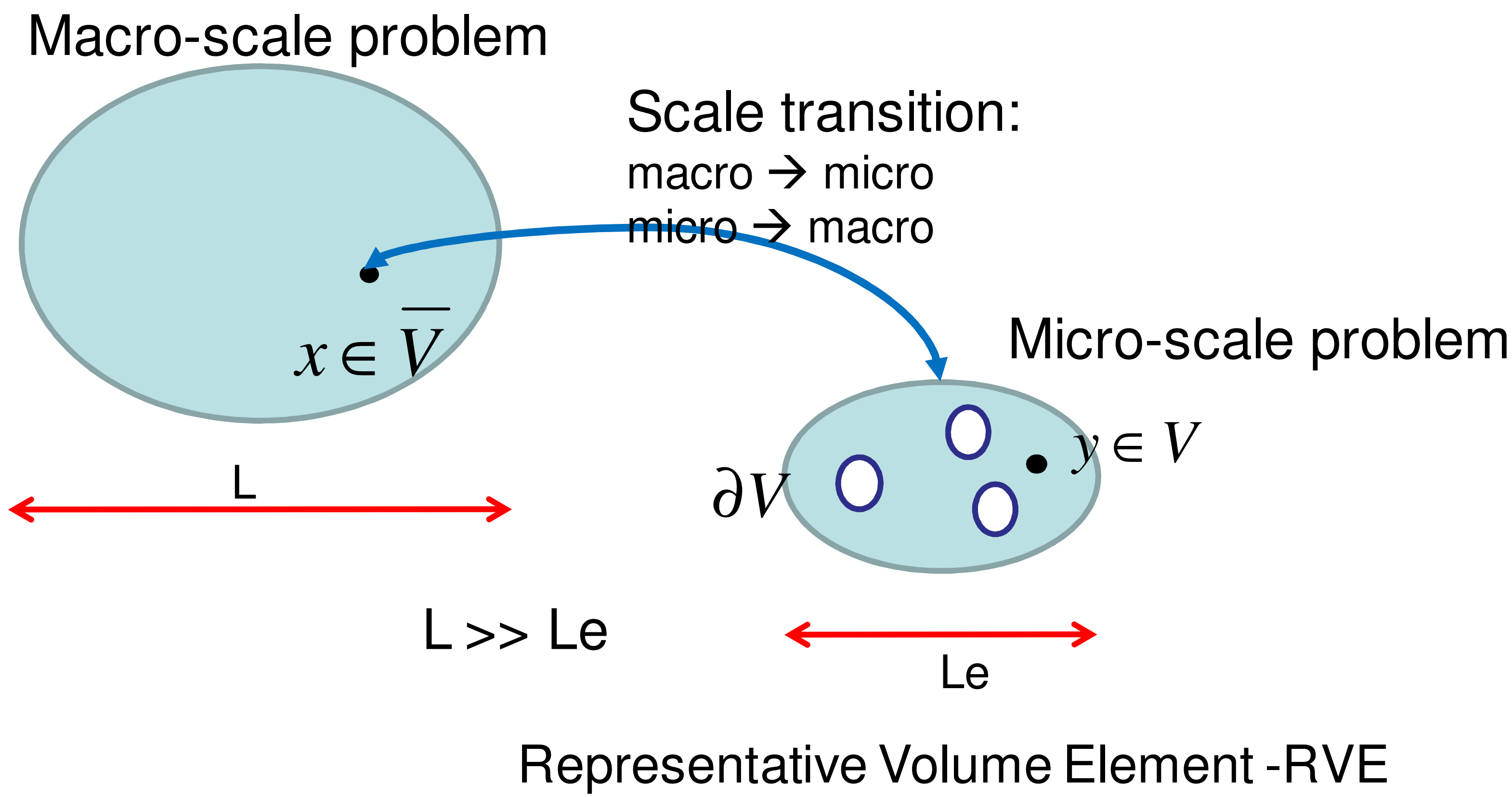
Outline

- Introduction
- Periodic boundary condition (PBC)
- Imposing PBC by interpolation
- Polynomial interpolation
- Numerical examples
- Conclusion and perspective

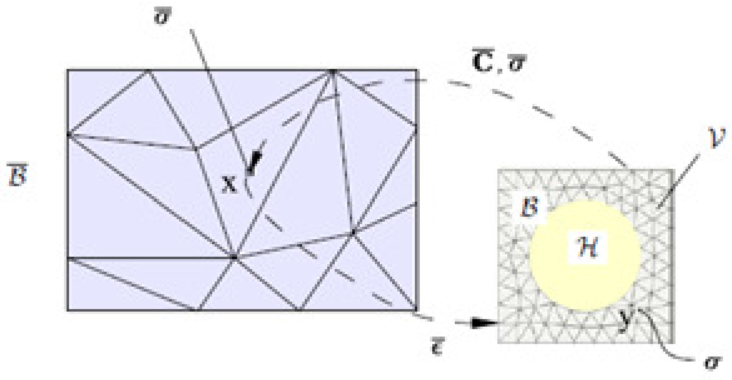
Introduction

- Multi-scale computational homogenization approach



Introduction

- Macro –variables and micro- variables
  - Micro-variables
    - Equilibrium state $div(\sigma) + \rho b = 0$
    - Micro- strain $\varepsilon = \nabla_s u$
    - Material law $\sigma = \hat{\sigma}(\varepsilon, \alpha, y)$



  - Macro-variables: averaging theory

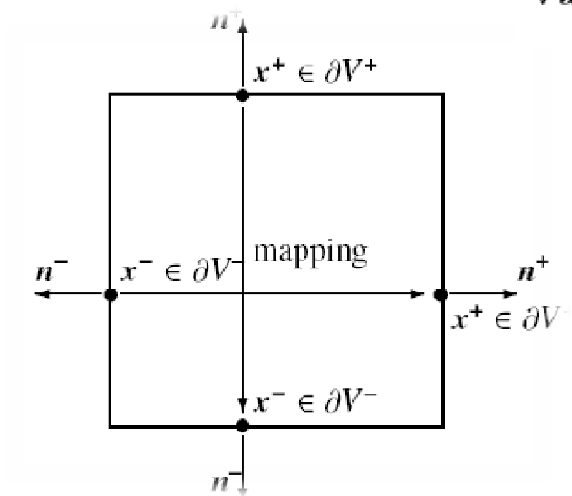
$$\bar{\sigma} = \frac{1}{V}\int_V \sigma dV \qquad \bar{\varepsilon} = \frac{1}{V}\int_V \varepsilon dV \qquad \bar{C} = \frac{d\bar{\sigma}}{d\bar{\varepsilon}}$$

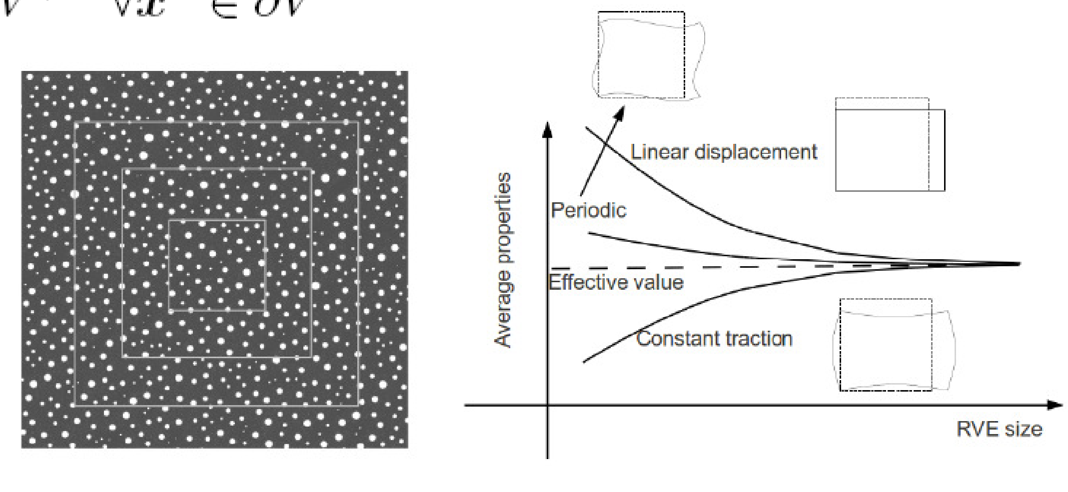
  - Hill-Mandel condition $\bar{\sigma} : \bar{\varepsilon} = \dfrac{1}{V}\displaystyle\int_V \sigma : \varepsilon dV$
  - Boundary condition at micro-scale must be defined in order to satisfy Hill-Mandel and kinematic averaging condition

Introduction

- Boundary value problem at micro-scale
  - Representative volume element (RVE)
  - Boundary conditions (BC) at micro-scale
    - Linear displacement BC: $\tilde{u}_i = u_i - \bar{\varepsilon}_{ij} x_j = 0 \qquad \forall \boldsymbol{x} \in \partial V$
    - Constant traction BC: $t_i = \bar{\sigma}_{ij} n_j \qquad \forall \boldsymbol{x} \in \partial V$
    - Periodic BC:

$$u_i^+ - u_i^- = \bar{\varepsilon}_{ij}(x_j^+ - x_j^-)$$
$$t_i^+ = -t_i^-$$
$$\forall \boldsymbol{x}^+ \in \partial V^+ \quad \forall \boldsymbol{x}^- \in \partial V^-$$

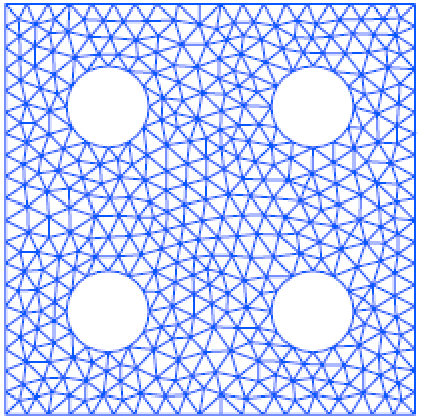


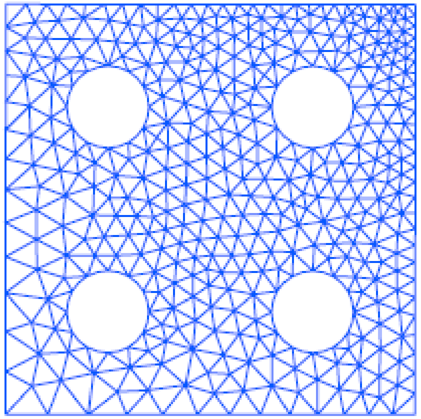


(a) (b)

Periodic boundary condition

- Compare with linear displacement BC and constant traction BC:
  - Better estimation for a RVE size
  - More effective in terms of convergent rate
- Implementation in finite element context
  - Periodic mesh (left image): easy by constraining on matching nodes
  - Non-periodic mesh (right image): difficult →**work objective**





Periodic boundary condition

- Imposing PBC by polynomial interpolation
  - Easy to implement
  - Applicable for arbitrary meshes
  - Applicable for 2-dimensional and 3-dimentional cases
  - Allows to impose strongly the PBC from the “weakest constraint” (linear displacement boundary condition) corresponding to the polynomial order 1 to the “strongest constraint” (classical PBC) corresponding to the polynomial high enough order.

Imposing PBC by interpolation

- Method idea
  - Displacement field of two opposite RVE sides is interpolated by linear combinations of some shape functions.

$$\boldsymbol{u}(\boldsymbol{s}) = \mathbb{S}(\boldsymbol{s}) = \sum_{i=0}^{n} \mathbb{N}_i(\boldsymbol{s})\boldsymbol{a}_i$$

  - Degrees of freedom of two opposite RVE sides are then substituted by the coefficients of these shape functions
- For imposing PBC
  - Displacement on negative part → interpolation form
  - Displacement form on positive part →PBC condition

$$\begin{aligned} \boldsymbol{u}_-(\boldsymbol{s}) &= \mathbb{S}(\boldsymbol{s})\,, \text{ and} \\ \boldsymbol{u}_+(\boldsymbol{s}) &= \mathbb{S}(\boldsymbol{s}) + \bar{\varepsilon}.(\boldsymbol{x}^+ - \boldsymbol{x}^-) \end{aligned}$$

- All DOFs on RVE boundary →interpolation coefficients **a**

Imposing PBC by interpolation

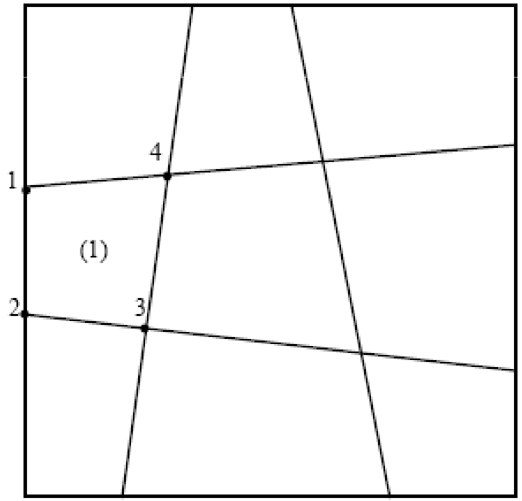
- Finite element implementation:
  - From interpolation form
    - Displacement on negative part $\boldsymbol{u}_{-} \quad = \quad \tilde{\mathbb{N}}\tilde{\boldsymbol{q}}$
    - Displacement on positive part $\boldsymbol{u}_{+} \quad = \quad \tilde{\mathbb{N}}\tilde{\boldsymbol{q}} + \bar{\varepsilon}(\boldsymbol{x}^{+} - \boldsymbol{x}^{-})$
    -
    - Shape function matrix $\tilde{\mathbb{N}}$ → user parameter
    - Coefficient matrix $\tilde{\boldsymbol{q}}$ → new DOFs add to systems

Imposing PBC by interpolation

- Finite element implementation:
  - Imposing PBC in element level
    - For element 1

$$\begin{aligned} \boldsymbol{u}_e(x,y) &= N_1(x,y)\boldsymbol{u}_1 + N_2(x,y)\boldsymbol{u}_2 + N_3(x,y)\boldsymbol{u}_3 + N_4(x,y)\boldsymbol{u}_4 = \mathbb{N}_e \boldsymbol{q}_e \\ \boldsymbol{q}_e^T &= \begin{bmatrix} \boldsymbol{u}_1^T & \boldsymbol{u}_2^T & \boldsymbol{u}_3^T & \boldsymbol{u}_4^T \end{bmatrix}. \end{aligned}$$

    - Node 1, 2 on RVE boundary
      - Negative part $\boldsymbol{u}_1 = \mathbb{N}_1 \tilde{\boldsymbol{q}}$, $\boldsymbol{u}_2 = \mathbb{N}_2 \tilde{\boldsymbol{q}}$
      - Positive part $\boldsymbol{u}_1 = \mathbb{N}_1 \tilde{\boldsymbol{q}} + \bar{\varepsilon}(\boldsymbol{x}^+ - \boldsymbol{x}^-)$, $\boldsymbol{u}_2 = \mathbb{N}_2 \tilde{\boldsymbol{q}} + \bar{\varepsilon}(\boldsymbol{x}^+ - \boldsymbol{x}^-)$



    - Element displacement vector

$$\boldsymbol{q}_e = \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{u}_2 \\ \boldsymbol{u}_3 \\ \boldsymbol{u}_4 \end{bmatrix} = \begin{bmatrix} \mathbb{N}_1 \tilde{\boldsymbol{q}} + \langle \boldsymbol{g} \rangle \\ \mathbb{N}_2 \tilde{\boldsymbol{q}} + \langle \boldsymbol{g} \rangle \\ \boldsymbol{u}_3 \\ \boldsymbol{u}_4 \end{bmatrix} = \mathbb{L}_e \tilde{\boldsymbol{q}}_e + \tilde{\boldsymbol{g}}_e$$

Imposing PBC by interpolation

- Finite element implementation:
  - Imposing PBC in element level
    - Finite element equations without constraints

$$\sum_e \left(\delta \boldsymbol{q}_e^T \boldsymbol{K}_e \boldsymbol{q}_e\right) - \sum_e \left(\delta \boldsymbol{q}_e^T \boldsymbol{F}_e\right) = 0$$

    - Element displacement constraints $\delta \boldsymbol{q}_e = \mathbb{L}_e \delta \tilde{\boldsymbol{q}}_e$
    - Finite element equation with constraints

$$\sum_e \left(\delta \tilde{\boldsymbol{q}}_e^T \mathbb{L}_e^T \boldsymbol{K}_e \mathbb{L}_e \tilde{\boldsymbol{q}}_e\right) - \sum_e \left(\delta \tilde{\boldsymbol{q}}_e^T \mathbb{L}_e^T \boldsymbol{F}_e - \delta \tilde{\boldsymbol{q}}_e^T \mathbb{L}_e^T \boldsymbol{K}_e \tilde{\boldsymbol{g}}_e\right) = 0$$

$$\sum_e \delta \tilde{\boldsymbol{q}}_e^T \left(\tilde{\boldsymbol{K}}_e \tilde{\boldsymbol{q}}_e - \tilde{\boldsymbol{F}}_e\right) = 0\,,$$

    - Modified element stiffness $\tilde{\boldsymbol{K}}_e = \mathbb{L}_e^T \boldsymbol{K}_e \mathbb{L}_e$
    - Modified external element force vector $\tilde{\boldsymbol{F}}_e = \mathbb{L}_e^T \left(\boldsymbol{F}_e - \boldsymbol{K}_e \tilde{\boldsymbol{g}}_e\right)$

Polynomial interpolation

- 2 –dimensional interpolation
  - Lagrange interpolation: global interpolation $\mathbb{S}(s) = \sum_{i=0}^{n} \boldsymbol{a}_i s^i$
    - Lagrange interpolation function

$$\boldsymbol{u} = \mathbb{S}(s) = \sum_{i=0}^{n} l_i(s)\boldsymbol{u}_i \qquad l_i(s) = \prod_{j=0, j\neq i}^{n} \frac{s - s_j}{s_i - s_j}$$

    - Matrix form $\boldsymbol{u}(s) = \tilde{\mathbb{N}}(s)\tilde{\boldsymbol{q}} \quad \tilde{\boldsymbol{q}}^T = [\boldsymbol{u}_0^T ... \boldsymbol{u}_n^T]$
    - If n =1, linear displacement BC is recovered.
  - Cubic spline interpolation: segment interpolation
    - Divide to segments $[(s_{i-1}, \boldsymbol{u}_{i-1}) \quad (s_i, \boldsymbol{u}_i)]$
    - Add slope to segment extremities $\boldsymbol{\theta}_{i-1}, \boldsymbol{\theta}_i$
    - Hermit interpolation function of order 3

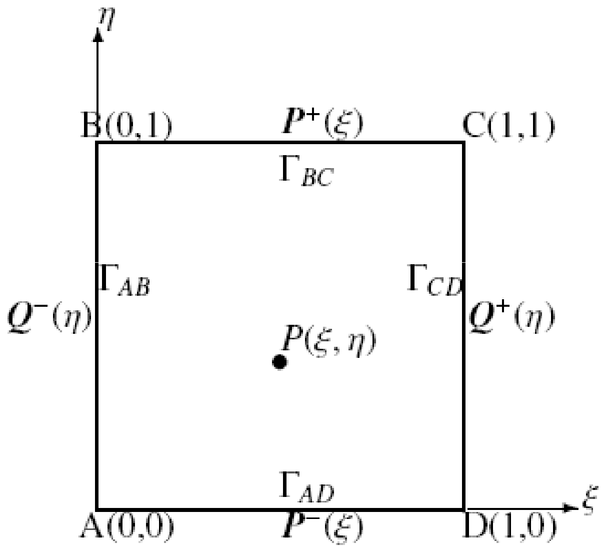
$$\boldsymbol{u}(s) = H_1(\xi(s))\boldsymbol{u}_{i-1} + H_2(\xi(s))\boldsymbol{\theta}_{i-1} + H_3(\xi(s))\boldsymbol{u}_i + H_4(\xi(s))\boldsymbol{\theta}_i$$

    - Matrix form $\boldsymbol{u}(s) = \tilde{\mathbb{N}}(\xi)\tilde{\boldsymbol{q}} \quad \tilde{\boldsymbol{q}}^T = [\boldsymbol{u}_0^T \boldsymbol{\theta}_0^T ... \boldsymbol{u}_N^T \boldsymbol{\theta}_N^T]$

Polynomial interpolation

- 3 –dimensional interpolation
  - Patch Coons interpolation
    - Displacement on edge → use 2-dimensional interpolation

$$\boldsymbol{Q}^{-}(\eta),\ \boldsymbol{P}^{-}(\xi),\ \boldsymbol{Q}^{+}(\eta) \text{ and } \boldsymbol{P}^{+}(\xi)$$



    - Displacement of interior nodes
    - → patch Coons formulation

$$\mathbb{S}_b(\xi,\eta) = \boldsymbol{S}_b^1(\xi,\eta) + \boldsymbol{S}_b^2(\xi,\eta) - \boldsymbol{S}_b^3(\xi,\eta)$$

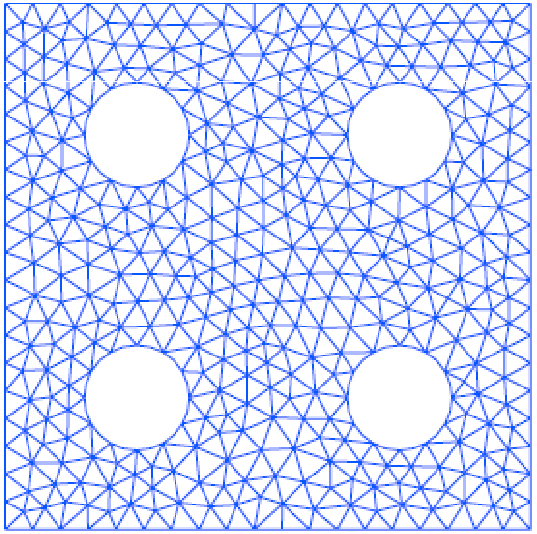
$$\boldsymbol{u}(\xi,\eta) = \mathbb{S}_b(\xi,\eta)$$

$$\begin{aligned}
\boldsymbol{S}_b^1(\xi,\eta) &= (1-\eta)\boldsymbol{P}^{-}(\xi) + \eta\boldsymbol{P}^{+}(\xi)\,, \\
\boldsymbol{S}_b^2(\xi,\eta) &= (1-\xi)\boldsymbol{Q}^{-}(\eta) + \xi\boldsymbol{Q}^{+}(\eta)\,, \text{ and} \\
\boldsymbol{S}_b^3(\xi,\eta) &= (1-\xi)(1-\eta)\boldsymbol{u}_A + (1-\xi)\eta\boldsymbol{u}_B + \xi\eta\boldsymbol{u}_C + \xi(1-\eta)\boldsymbol{u}_D
\end{aligned}$$

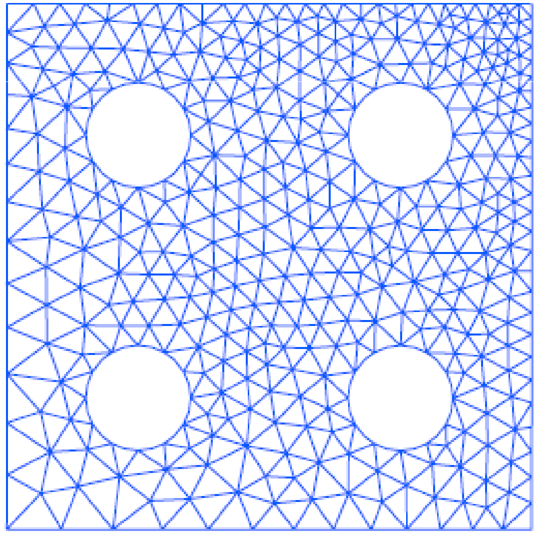
    - By some manipulations $\boldsymbol{u}(\xi,\eta) = \boldsymbol{P}^{-}(\xi) + \boldsymbol{Q}^{-}(\eta) - \boldsymbol{u}_A$
    - By matrix form $\boldsymbol{u}(\xi,\eta) = \tilde{\mathbb{N}}_P(\xi)\tilde{\boldsymbol{q}}_P + \tilde{\mathbb{N}}_Q(\eta)\tilde{\boldsymbol{q}}_Q = \tilde{\mathbb{N}}(\xi,\eta)\tilde{\boldsymbol{q}}$

Numerical examples

- 2 –dimensional cases
  - Elastic material E = 70GPa, Poisson ration = 0.3
  - Plan strain state and small deformation
  - With periodic hole structures: PBC with matching node and with polynomial interpolation → Method validation



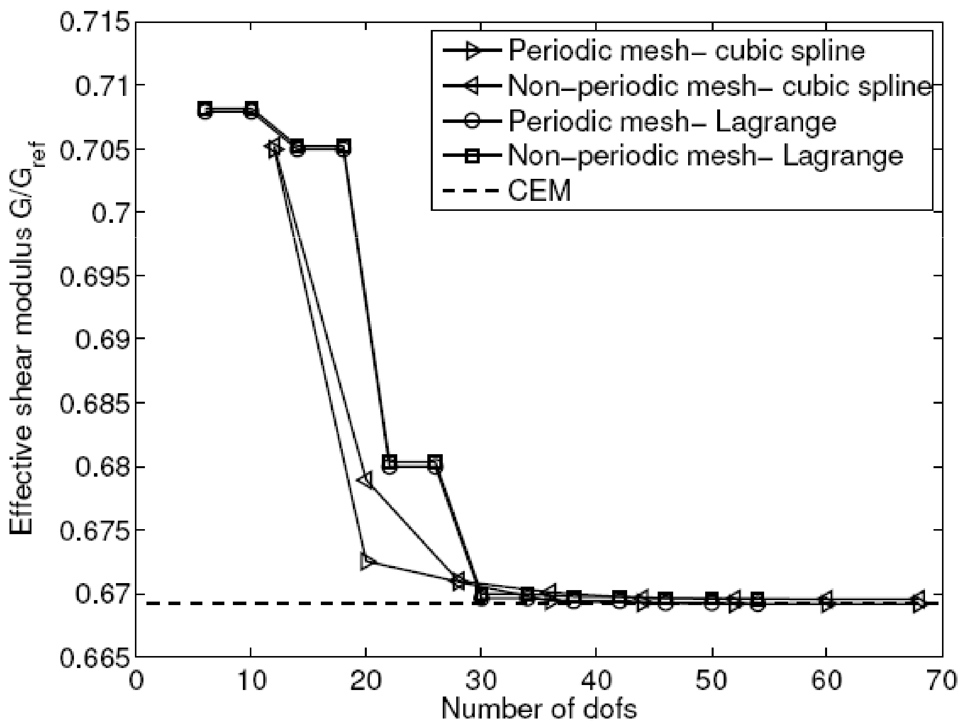
Periodic mesh
from periodic materials



Non-periodic mesh
from periodic materials

Numerical examples

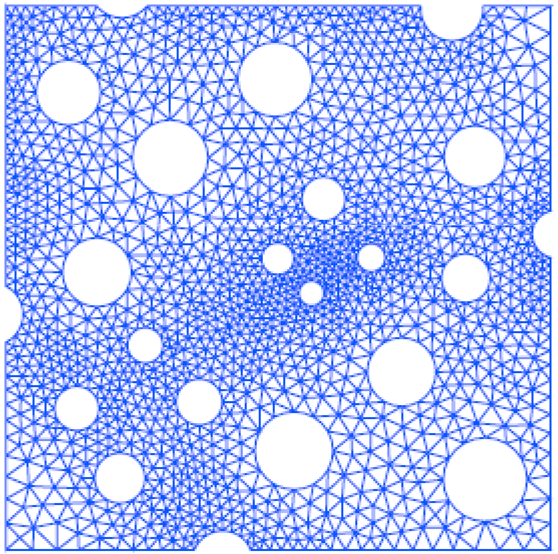
- 2 –dimensional cases
  - With periodic hole structures
    - CEM = constraint elimination method for periodic mesh



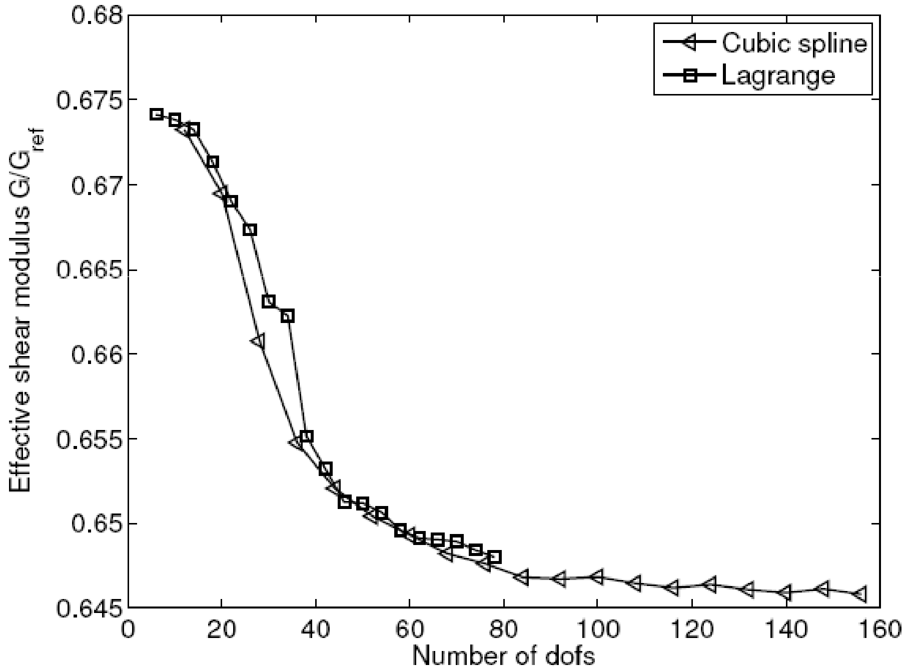
Convergence of effective property in terms of new DOFs added to system

Numerical examples

- 2 –dimensional cases
  - With random hole structures: non-periodic mesh
    - → method efficiency



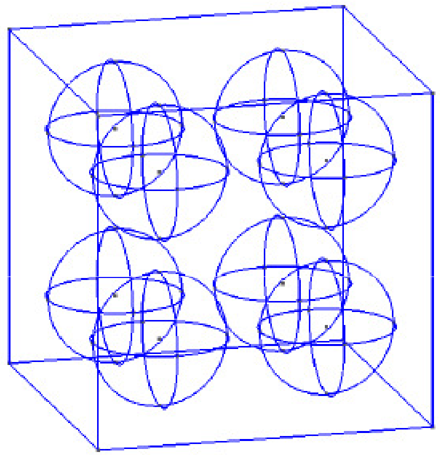
Non-periodic mesh
from random materials

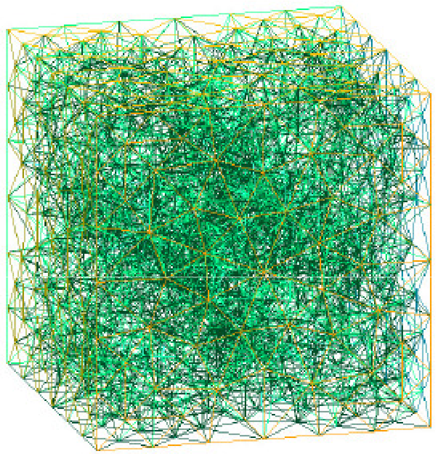


Convergence of effective property in terms of new DOFs added to system

Numerical examples

- 3 –dimensional cases
  - With periodic structure: periodic mesh
    - Lagrange:
      - order 5
    - Cubic spline:
      - 5 segments





$$\bar{\boldsymbol{\varepsilon}} = \begin{bmatrix} 0.01 & 0.005 & 0.005 \\ 0.005 & 0.01 & 0.005 \\ 0.005 & 0.005 & 0.01 \end{bmatrix}$$

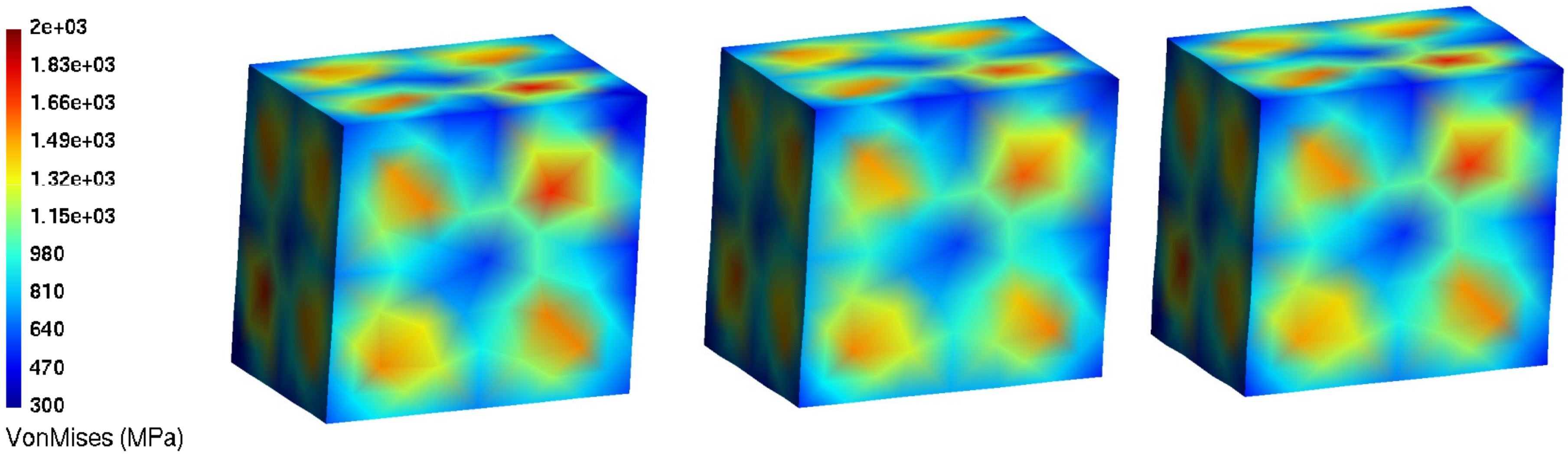
$$\bar{\sigma}_{\text{CEM}} = \begin{bmatrix} 984.801 & 164.761 & 165.98 \\ 164.761 & 985.002 & 164.653 \\ 165.98 & 164.653 & 984.876 \end{bmatrix} \text{MPa}$$

$$\bar{\sigma}_{\text{Lagrange}} = \begin{bmatrix} 988.71 & 167.202 & 168.302 \\ 167.202 & 988.812 & 167.646 \\ 168.302 & 167.646 & 988.572 \end{bmatrix} \text{MPa}$$

$$\bar{\sigma}_{\text{spline}} = \begin{bmatrix} 986.437 & 166.003 & 167.221 \\ 166.003 & 986.534 & 166.254 \\ 167.221 & 166.254 & 986.341 \end{bmatrix} \text{MPa}$$

Numerical examples

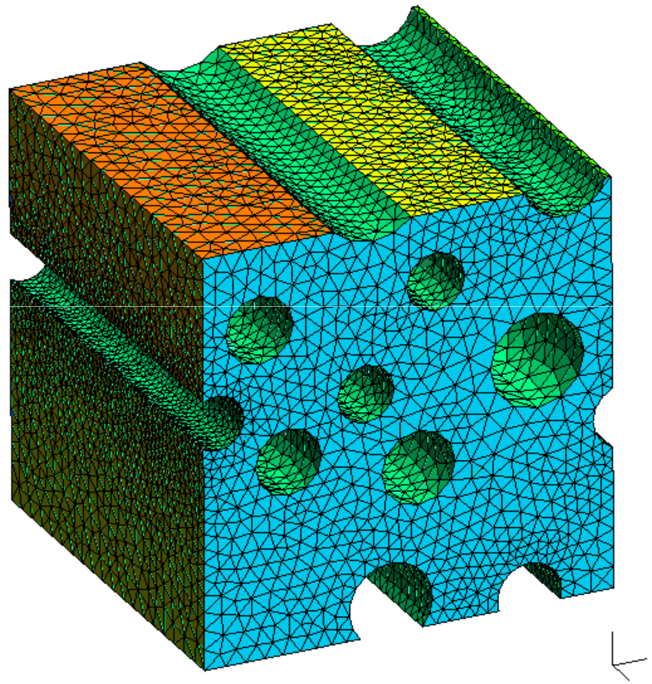
- 3 –dimensional cases
  - With periodic structure: periodic mesh
    - Von-Mises stress distribution



CEM Lagrange Cubic spline

Numerical examples

- 3 –dimensional cases
  - With random structure: non- periodic mesh
    - Lagrange:
      - order 15
    - Cubic spline:
      - 10 segments



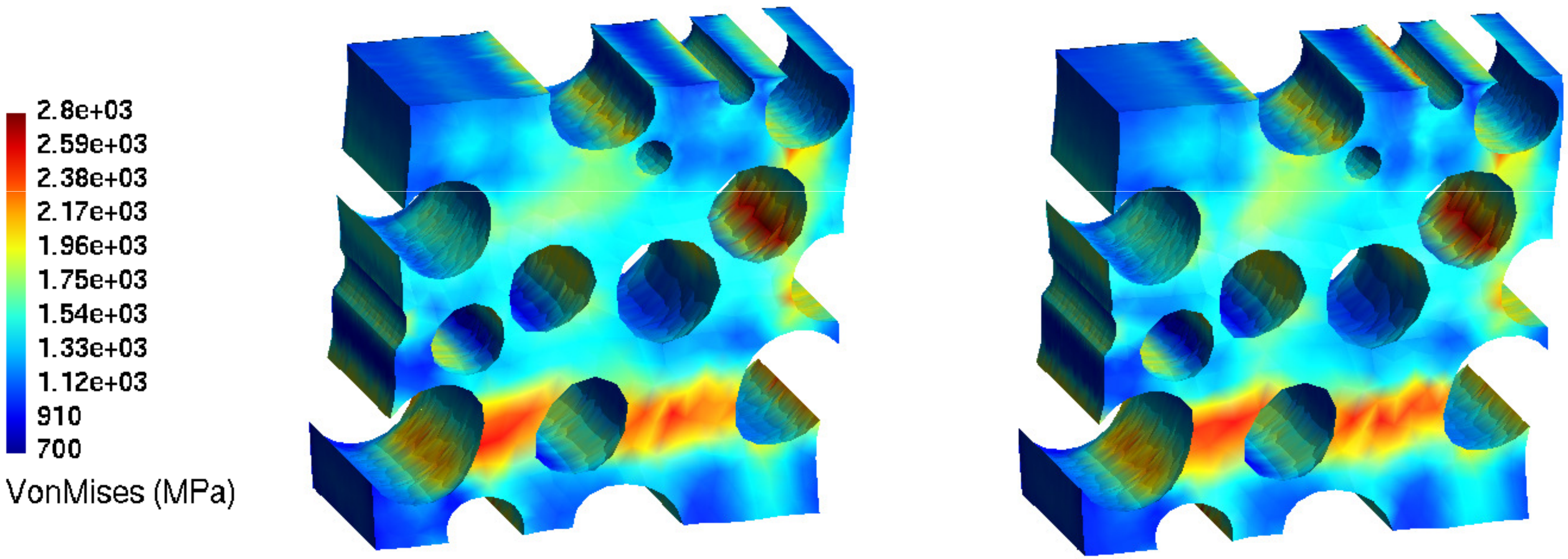
$$\bar{\varepsilon} = \begin{bmatrix} 0.01 & 0.005 & 0.005 \\ 0.005 & 0.01 & -0.005 \\ 0.005 & -0.005 & -0.01 \end{bmatrix}$$

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

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

Numerical examples

- 3 –dimensional cases
  - With random structure: non- periodic mesh
    - Von-Mises stress distribution



Lagrange

Cubic spline

Conclusion and perspective

- Conclusion
  - A new method to enforce the PBC is presented
    - By using interpolation formulation
    - For arbitrary meshes
    - For 2-dimensional and 3-dimensional cases
    - Better estimation in compared with linear displacement BC which usually uses for non-periodic meshes
  - Key advantage of this method is the elimination of the need of matching nodes
  - Some examples demonstrated the method efficiency.
- Perspective
  - Study effective properties of foams by using periodic boundary condition