Alternative numerical method in continuum mechanics

COMPUTATIONAL MULTISCALE

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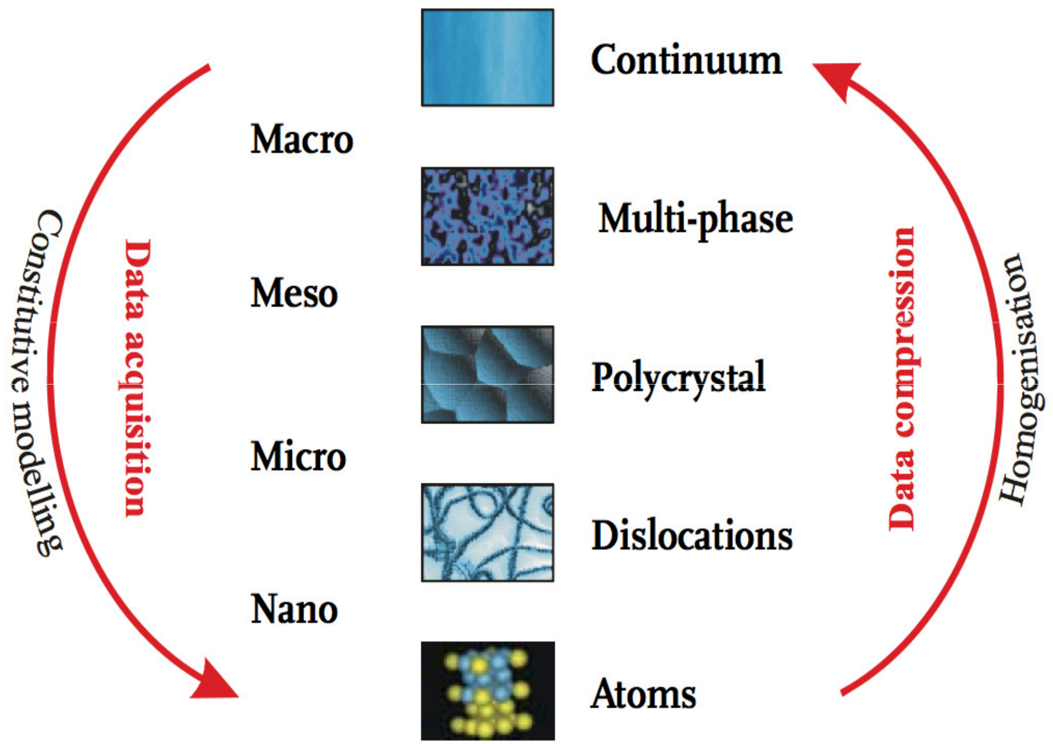
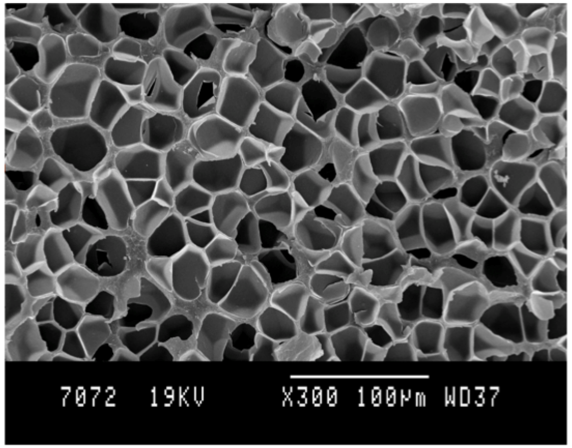
Content

Scales of complex micro-structured materials



Scales of complex micro-structured materials



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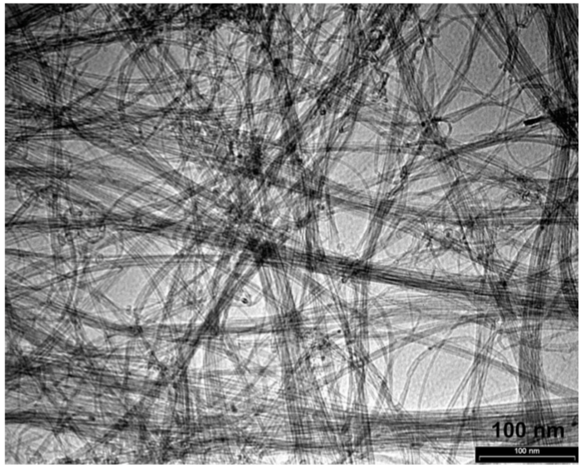


Carbon nanotubes

manufactured by nanocyl

Classification of multiscale methods

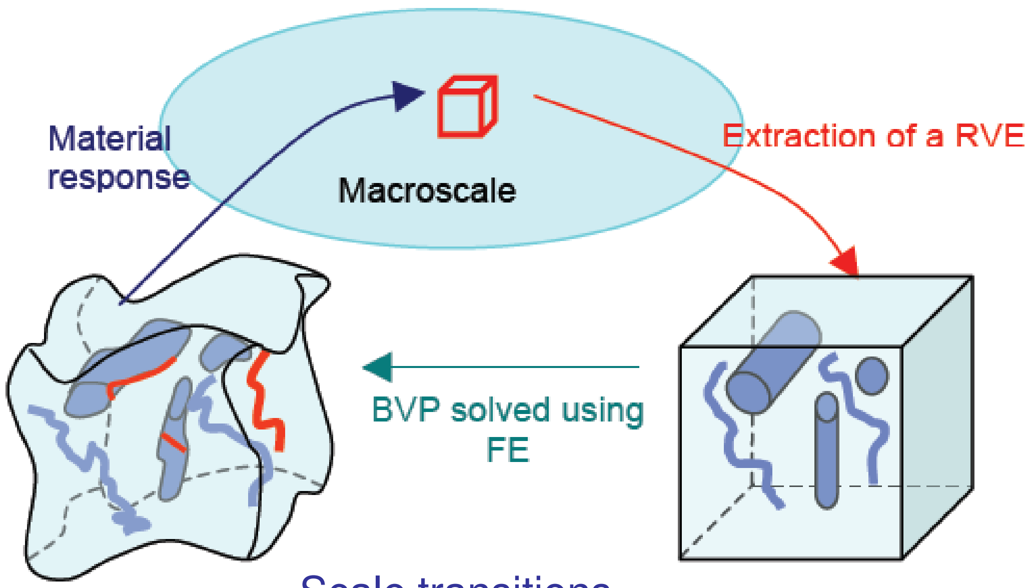
- Multiscale problems can be divided into two classes :
  - Type A problems : deal with isolated defects near which the macroscopic models are invalid (shocks, cracks, dislocations,…). Elsewhere the explicitly given macroscale model is valid.
  - Type B problems : constitutive modeling is based on the microscopic models for which the macroscopic model is not explicitly available and is instead determined from the microscopic model.
- **Heterogeneous Multiscale Method (HMM)** has been attempting to build a unified framework for designing effective simulation methods that couple microscale and macroscale models. HMM applies for both type A and type B problems
- In general, there is no restriction on models that can be used at both macroscale and microscale (continuum media, molecular dynamics, quantum physics,…).
- In this presentation, we restrict ourselves to type B problems. We also consider continuum media models at both scales.

Computational multiscale methods allow to model complex micro-structured materials using more accurate macroscopic constitutive laws.

- The heterogeneous nature and the multiscale structure of complex micro-structured materials confer them some remarkable properties:
  - mechanical: resistance, increased Young modulus, negative Poisson ratio…
  - electromagnetic/optic: resistance, electromagnetic shielding, $\mu < 0$, $\varepsilon < 0$…
- Classical methods are not efficient to model these materials :
  - direct simulation methods such as the finite element method are costly in terms of computational time and memory.
  - the trial-and-error approach that consists in manufacturing the material and then measure its physical properties is costly and not suited for optimization.
- Computational methods have been succesfully used to model complex micro-structured materials :
  - for linear/slightly nonlinear materials,the Mean-Field Homogenization method is efficient.
  - for highly nonlinear complex micro-structured materials, all other methods fail and only Computational Multiscale Methods (CMM) remain valid.

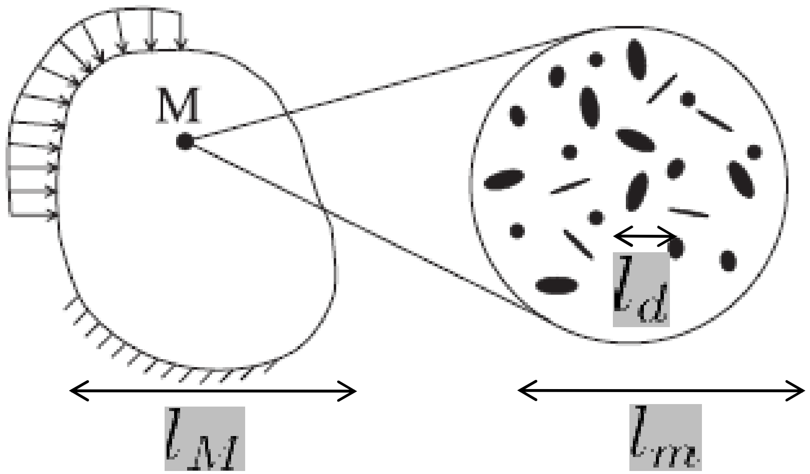
CMM – macro/micro-problems and scale transitions

- In the CMM framework, 2 problems are defined:
  - Macroscale problem
  - Microscale problem (Boundary Value Problem- BVP)
- Scale transitions allow coupling two scales :
  - upscaling: constitutive law (e.g.: stress, tangent operator) for macroscale problem is determined from microscale problem (e.g. using averaging theory).
  - downscaling: transfer of macroscale quantities (e.g.: strain) to the microscale. These quantities allow determining equilibrium state of BVP.



Scale transitions

- Material macroscopically sufficiently homogeneous, but microscopically heterogeneous (inclusions, grains, interfaces, cavities,…) → (continuum media and averaging theorems).
- **Scale separation**: the characteristic at microscale must be much smaller than the characteristic size at macroscale.
- Two additional assumptions can be made:
  - The characteristic size of the heterogeneities must be much greater than the molecular dimension (continuum media at the microscale).
  - The characteristic size of the heterogeneities must be much smaller than the size of the RVE (RVE statistically representative).



$$l_a \ll l_d \ll l_m \ll l_M$$

Heterogeneous micro-structure associated with macroscopic continuum point M

Computational Multiscale Method – advantages

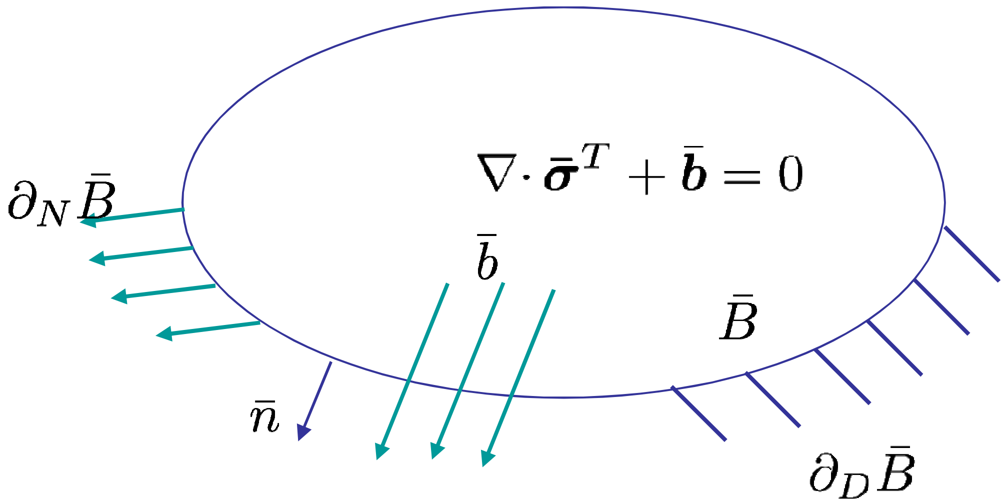
Some key advantages:

– Do not require any constitutive assumption with respect to the overall material behavior.
– Enable the incorporation of large deformations and rotations on both micro and macro-level.
– Are suitable for arbitrary material behavior, including physically non-linear and time dependent behavior.
– Provide the possibility to introduce detailed micro-structural information, including a physical and/or geometrical evolution of the microstructure, in the macroscopic analysis.
– Allow the use of any modeling technique at the micro-level.
– Microscale problems are solved independently from each others and the method can be easily parallelized.

History

- Approaches to solve scale transitions problems:
  - 1965: Method based on Eshelby results: Mean-field homogenization (Hill)
  - 1978: Asymptotic homogenization method (A. Bensoussan et al.)
  - 1985: Global-local method (Suquet).
  - 1995: First-order computational homogenization method (Ghosh et al.)
  - 2001: Extension to the second-order (Geers et al.)
  - 2003: Heterogeneous Multiscale Method - HMM (E et al.).
  - 2007: Continuous–discontinuous multiscale approach (Massart et al.) and computational homogenization of thin sheets and shells (Geers et al)
  - 2008: Thermo-mechanical coupling (Ozdemir et al.) and Computational homogenization of interface problems (Matous et al)
- Applications:
  - Mechanics: damage and fracture analysis, thin sheet and shells, failure analysis of cohesive interfaces, flow transport through heterogeneous porous media…
  - Heat transfer: heat conduction in heterogeneous media

- Macroscopic problem

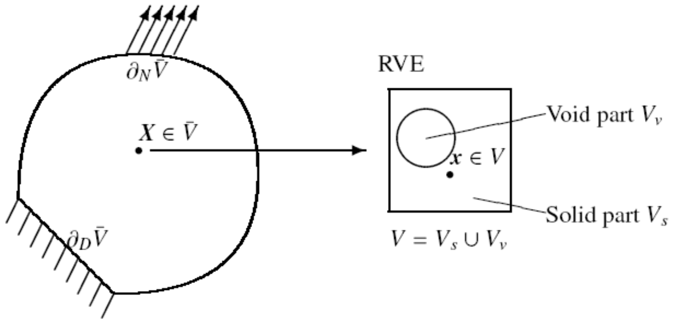


  - Weak form

$$\int_{\bar{B}} \bar{\boldsymbol{\sigma}} : \nabla \delta \varphi \, dV = \int_{\partial_N \bar{B}} \bar{\boldsymbol{T}} : \nabla \delta \varphi \, dS + \int_{\bar{B}} \bar{\boldsymbol{b}} : \nabla \delta \varphi \, dV$$

Definition of microscopic problem

- Representative volume element (RVE)
  - A model of material micro-structure which is used to obtain the macroscopic material response at a macroscopic material point.



RVE associated with a macroscopic point

- Selection of RVE
  - RVE contains all necessary information of micro-structure
  - Computation efficiency
- RVE equilibrium state
  - In absence of body forces: $\nabla.\boldsymbol{\sigma}^T = 0$
  - Constitutive law: $\boldsymbol{\sigma}^{(i)} = \mathcal{F}_i(\boldsymbol{\varepsilon})$
  - For hyper-elastic material $\boldsymbol{\sigma} = \partial_{\boldsymbol{\varepsilon}} W$
  - Equilibrium state of the RVE is assumed to be consistent with the boundary condition, which are related to the macroscopic strain field

- Boundary condition
  - Strain driven problem
  - Microscopic strain: $\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \otimes \boldsymbol{u} + \boldsymbol{u} \otimes \nabla) = \nabla \otimes_s \boldsymbol{u}$
  - Macroscopic strain:

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V}\int_V \boldsymbol{\varepsilon}\, dV$$

  - Using Gauss theorem: $\bar{\boldsymbol{\varepsilon}} = \frac{1}{V}\oint_{\partial V} \boldsymbol{n} \otimes_s \boldsymbol{u}\, dS$

$$\frac{1}{V}\oint_{\partial V} \boldsymbol{n} \otimes_s (\boldsymbol{u} - \bar{\boldsymbol{\varepsilon}}\boldsymbol{x})\, dS = 0$$

  - Split of displacement field: mean part and fluctuation part:

$$\boldsymbol{u} = \bar{\boldsymbol{u}} + \tilde{\boldsymbol{u}} = \bar{\boldsymbol{\varepsilon}}\boldsymbol{x} + \tilde{\boldsymbol{u}} \qquad \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} + \nabla \otimes_s \tilde{\boldsymbol{u}} \qquad \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} + \tilde{\boldsymbol{\varepsilon}}$$

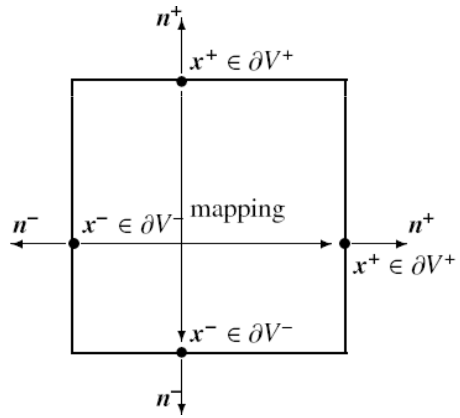
  - Constrain on the fluctuation field: $\frac{1}{V}\oint_{\partial V} \boldsymbol{n} \otimes_s \tilde{\boldsymbol{u}}\, dS = 0$ (*)
  - Boundary condition must be defined to satisfy (*)

- Boundary condition
  - Hill assumption (rule of mixtures): no fluctuations in RVE
  - Linear displacement boundary condition (Dirichlet boundary condition): no fluctuation at RVE boundary

$$\tilde{\boldsymbol{u}} = 0 \qquad \forall \boldsymbol{x} \in \partial V$$

  - Periodic boundary condition: periodicity of fluctuation field and anti-periodicity of traction field at RVE boundary

$$\tilde{\boldsymbol{u}}^+ = \tilde{\boldsymbol{u}}^- \qquad \forall \boldsymbol{x}^+ \in \partial V^+ \text{ and } \forall \boldsymbol{x}^- \in \partial V^-$$
$$\boldsymbol{t}^+ = -\boldsymbol{t}^- \qquad \boldsymbol{n}^+ = -\boldsymbol{n}^-$$

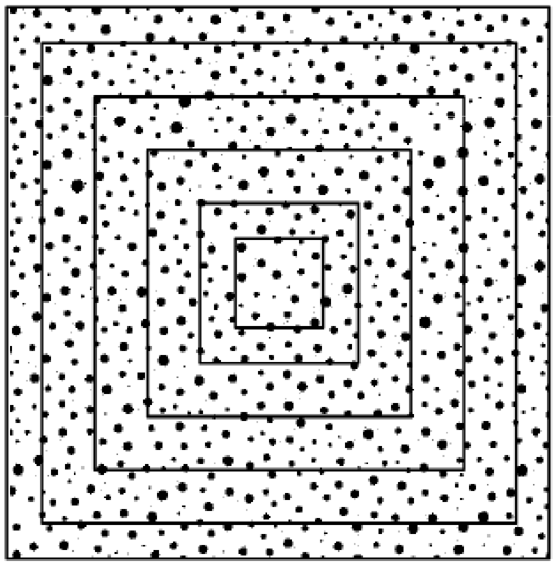


  - Minimal kinematic boundary condition (Neumann boundary condition)

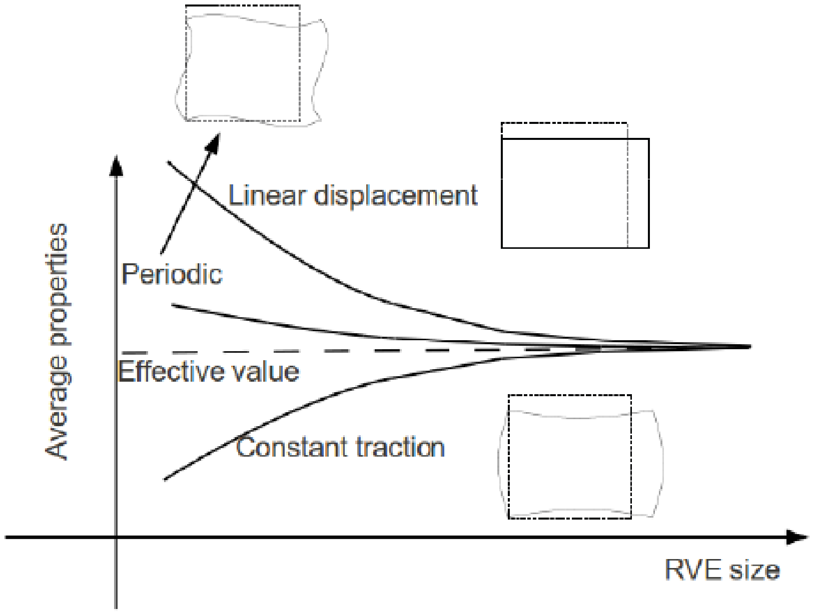
$$\boldsymbol{t} = \bar{\boldsymbol{\sigma}}.\boldsymbol{n} \qquad \forall x \in \partial V$$

Definition of microscopic problem

- Boundary condition
  - Periodic boundary condition is the most efficient in terms of convergence rate
  - Linear displacement upper-estimate the effective properties
  - Constant traction (Neumann BC) under-estimate the effective properties



RVE selection



Convergence of average properties with increasing RVE size.

Coupling of microscopic and macroscopic problem

- Strain averaging

$$\bar{\varepsilon} = \frac{1}{V}\int_V \varepsilon \, dV \qquad \bar{\varepsilon} = \frac{1}{V}\oint_{\partial V} \boldsymbol{n} \otimes_s \boldsymbol{u} \, dS$$

- Hill-Mandel principle:
  - Energy consistency in the transition of macro- and micro-scales:

$$\delta \bar{W} = \frac{1}{V}\int_V \delta W \, dV \quad (**)$$

  - For elastic material in small strain: $\bar{\boldsymbol{\sigma}} : \delta\bar{\varepsilon} = \frac{1}{V}\int_V \boldsymbol{\sigma} : \delta\varepsilon \, dV$
  - Virtual strain: $\delta\varepsilon = \delta\bar{\varepsilon} + \delta\tilde{\varepsilon}$
  - Equation (**) becomes: $\bar{\boldsymbol{\sigma}} : \delta\bar{\varepsilon} = \frac{1}{V}\int_V \boldsymbol{\sigma} \, dV : \delta\bar{\varepsilon} + \frac{1}{V}\int_V \boldsymbol{\sigma} : \delta\tilde{\varepsilon} \, dV$
  - Stress averaging: $\bar{\boldsymbol{\sigma}} = \frac{1}{V}\int_V \boldsymbol{\sigma} \, dV$

Coupling of microscopic and macroscopic problem

- Hill-Mandel principle:
  - Hill-Mandel condition in terms of fluctuation part: $$\frac{1}{V}\int_V \boldsymbol{\sigma} : \delta\tilde{\boldsymbol{\varepsilon}}\, dV = 0$$
  - Using the equilibrium state and Gauss theorem: $$\frac{1}{V}\int_{\partial V} \boldsymbol{t}.\delta\tilde{\boldsymbol{u}}\, dS = 0 \qquad (***)$$
  - All boundary conditions previously defined satisfy the condition (***)

- Stress averaging and tangent operator
  - Equilibrium state and Gauss theorem:

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V}\int_V \boldsymbol{\sigma}\, dV \qquad \bar{\boldsymbol{\sigma}} = \frac{1}{V}\int_{\partial V} \boldsymbol{t} \otimes \boldsymbol{x}\, dS$$

  - Tangent operator: $\bar{\mathbf{C}} = \partial_{\bar{\varepsilon}} \bar{\boldsymbol{\sigma}}$

- Finite element model at microscopic scale
  - Minimal potential energy principle $$\bar{U} = \frac{1}{V}\int_V U \, dV$$
  - Discretize the displacement fluctuations at element level
$$\tilde{\boldsymbol{u}} = \boldsymbol{N}^e(x)\boldsymbol{q}_e$$
$$\tilde{\varepsilon} = \nabla \otimes_s \tilde{\boldsymbol{u}} = \boldsymbol{B}^e(x)\boldsymbol{q}_e$$
  - Assemble operator $\boldsymbol{q} = \mathcal{A}_{e=1}^{n_e}\boldsymbol{q}_e$
  - Approximation of internal energy: $$\bar{U}^h(\bar{\varepsilon}, \boldsymbol{q}) = \frac{1}{V}\mathcal{A}_{e=1}^{n_e}\int_{V_e} U(\bar{\varepsilon} + \boldsymbol{B}^e\boldsymbol{q}_e)\, dV$$

- RVE boundary condition
  - Linear displacement boundary condition
    - For M nodes on RVE boundary

$$\tilde{\boldsymbol{u}}_i = 0 \qquad i = 1..M$$

    - Partitioning of fluctuation field on RVE boundary

$$\boldsymbol{q}^T = [\boldsymbol{q}_i^T \, \boldsymbol{q}_b^T]$$
$$\boldsymbol{q}_i = \boldsymbol{L}_i \boldsymbol{q}$$
$$\boldsymbol{q}_b = \boldsymbol{L}_b \boldsymbol{q}$$

    - Linear constraints on fluctuation displacement

$$\boldsymbol{q}_b = 0$$
$$\boldsymbol{L}_b \boldsymbol{q} = 0$$

- RVE boundary condition
  - Constant traction boundary condition
    - From strain averaging equation

$$\frac{1}{V}\oint_{\partial V} \boldsymbol{n} \otimes_s \tilde{\boldsymbol{u}}\, dS = 0 \quad (*)$$

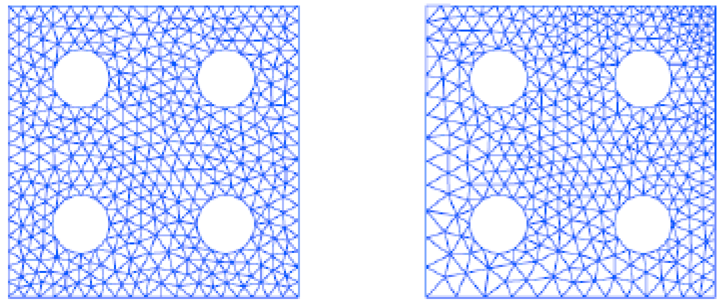
    - Assemble on RVE boundary elements

$$\frac{1}{V}\mathcal{A}_{e=1}^{n_e} \int_{(\partial V)_e} \boldsymbol{n} \otimes_s \boldsymbol{B}^e \boldsymbol{q}_e \, dS = 0$$

    - Linear constraints on fluctuation displacement

$$\boldsymbol{L}_b \boldsymbol{q} = 0$$

- RVE boundary condition
  - Periodic boundary condition
    - Periodic mesh requirement

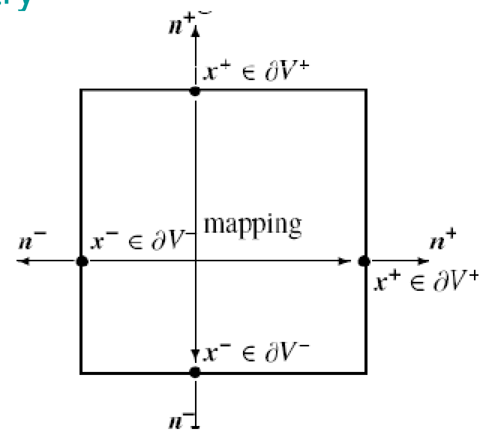


Periodic mesh and non-periodic mesh

- Periodic mesh: apply on matching node on RVE boundary

$$\tilde{\boldsymbol{u}}^{+} = \tilde{\boldsymbol{u}}^{-} \qquad \forall \boldsymbol{x}^{+} \in \partial V^{+} \text{ and } \forall \boldsymbol{x}^{-} \in \partial V^{-}$$

$$\boldsymbol{t}^{+} = -\boldsymbol{t}^{-} \qquad \boldsymbol{n}^{+} = -\boldsymbol{n}^{-}$$



Matching node

- Linear constraints on fluctuation displacement

$$\boldsymbol{q}^{+} = \boldsymbol{q}^{-}$$

$$\boldsymbol{C}_b q_b = 0$$

$$C_b \boldsymbol{L}_b \boldsymbol{q} = 0$$

$$\boldsymbol{C}\boldsymbol{q} = 0$$

- RVE boundary condition
  - Periodic boundary condition
    - Non-periodic mesh: polynomial interpolation method

$$u_- = N\tilde{q}$$

$$u_+ = N\tilde{q} + \bar{\varepsilon}(x_+ - x_-)$$

    - Linear constraints on fluctuation displacement

$$\boldsymbol{C}\boldsymbol{q} = 0$$

- RVE equilibrium state
  - Minimize $$\bar{U}^h(\bar{\varepsilon}, \boldsymbol{q}) = \frac{1}{V}\mathcal{A}_{e=1}^{n_e} \int_{V_e} U(\bar{\varepsilon} + \boldsymbol{B}^e \boldsymbol{q}_e)\, dV$$
  - Subject to: $$\boldsymbol{C}\boldsymbol{q} = \boldsymbol{g}$$

- Enforcement by Lagrange multipliers
  - Lagrange function $$\mathcal{L} = \bar{U}^h(\bar{\varepsilon}, \boldsymbol{q}) - \lambda^T(\boldsymbol{C}\boldsymbol{q} - \boldsymbol{g})$$
  - Equilibrium state $$\partial_q \bar{U}^h - \boldsymbol{C}^T \boldsymbol{\lambda} = 0$$ $$\boldsymbol{C}\boldsymbol{q} - \boldsymbol{g} = 0$$
  - Internal force $$\boldsymbol{F}_{\text{int}} = \partial_q \bar{U}^h$$
  - Nonlinear system $$\boldsymbol{F}_{\text{int}} - \boldsymbol{C}^T \boldsymbol{\lambda} = 0$$ $$\boldsymbol{C}\boldsymbol{q} - \boldsymbol{g} = 0$$

- Enforcement by Lagrange multipliers
  - Nonlinear system to solve $\boldsymbol{F}_{\text{int}} - \boldsymbol{C}^T \boldsymbol{\lambda} = 0$

    $\boldsymbol{C}\boldsymbol{q} - \boldsymbol{g} = 0$
  - Solve by Newton-Raphson procedure
    - Step 0 $\boldsymbol{q}^{(0)} = \boldsymbol{q}_0 \qquad \boldsymbol{\lambda}^{(0)} = \boldsymbol{\lambda}_0$
    - Step 1 $\begin{bmatrix} \Delta \boldsymbol{q}^{(i)} \\ \Delta \boldsymbol{\lambda}^{(i)} \end{bmatrix} = -\boldsymbol{S}_T^{-1} \begin{bmatrix} F_{\text{int}}^{(i)} - \boldsymbol{C}^T \boldsymbol{\lambda}^{(i)} \\ \boldsymbol{C}\boldsymbol{q}^{(i)} - \boldsymbol{g} \end{bmatrix} \qquad \boldsymbol{S}_T = \begin{bmatrix} \partial_q F_{\text{int}}^{(i)} & -\boldsymbol{C}^T \\ \boldsymbol{C} & 0 \end{bmatrix}$
    - Step 2 $\boldsymbol{q}^{(i+1)} = \boldsymbol{q}^{(i)} + \Delta \boldsymbol{q}^{(i)}$

      $\boldsymbol{\lambda}^{(i+1)} = \boldsymbol{\lambda}^{(i)} + \Delta \boldsymbol{\lambda}^{(i)}$
    - Step 3 $\boldsymbol{r}^{(i+1)} = \boldsymbol{F}_{\text{int}}^{(i+1)} - \boldsymbol{C}^T \boldsymbol{\lambda}^{(i+1)}$

      $\boldsymbol{\Phi}^{(i+1)} = \boldsymbol{C}\boldsymbol{q}^{(i+1)} - \boldsymbol{g}$
    - If $\max(||\boldsymbol{r}^{(i+1)}||, ||\boldsymbol{\Phi}^{(i+1)}||) < \text{tol}$ EXIT
    - else GOTO step 1

- Enforcement by constraint elimination
  - Problem:

$$\delta \boldsymbol{q}^T \left(\partial_q \bar{U}^h \right) = 0$$

  - Decomposition: dependent part and independent part from constraints

$$\delta \boldsymbol{q}^D = \boldsymbol{S} \delta \boldsymbol{q}^I \qquad \boldsymbol{q} = \begin{bmatrix} \boldsymbol{q}^I \\ \boldsymbol{q}^D \end{bmatrix} \qquad \delta \boldsymbol{q} = \boldsymbol{L} \delta \boldsymbol{q}^I$$

  - New equation of independent part

$$(\delta \boldsymbol{q}^I) \boldsymbol{L}^T F_{\text{int}}(\boldsymbol{q}^I) = 0$$

  - Solve by Newton-Raphon procedure

Nested solution scheme

MACRO

- Step 1: Initialization
  - Assign RVE to every integration points (IPs)
  - Set $\bar{\varepsilon} = 0$ for all Ips

$\xrightarrow{\bar{\varepsilon} = 0}$

$\xleftarrow{\bar{\mathcal{C}}}$

- Step 2: next load increment at macroscopic problem
- Step 3: next Iteration
  - Solve macroscopic problem
  - Calculate macroscopic forces

$\xrightarrow{\bar{\varepsilon}}$

$\xleftarrow{\bar{\sigma}}$

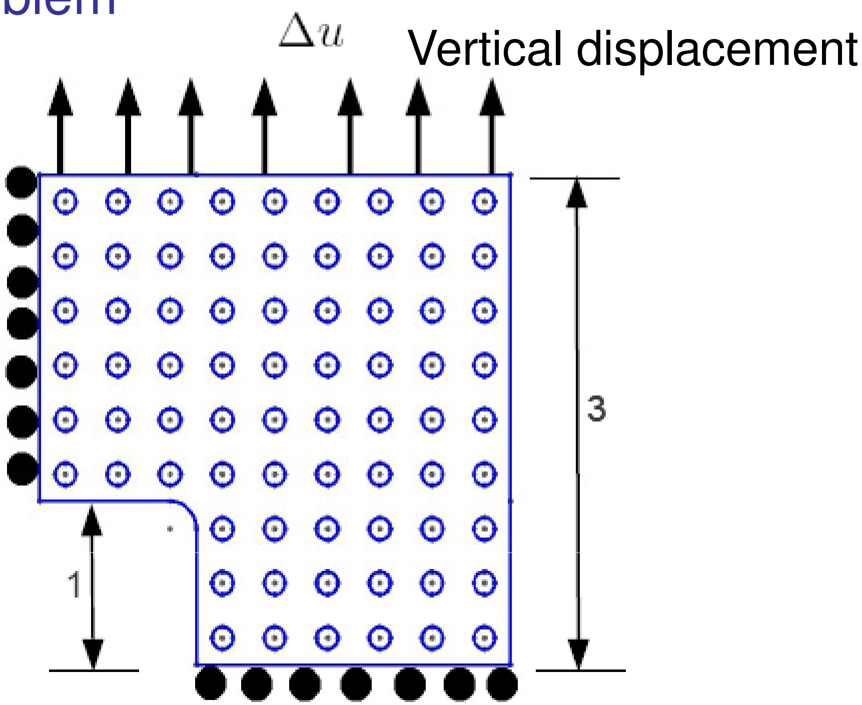
$\xleftarrow{\bar{\mathcal{C}}}$

- Step 4: convergence
  - If convergence → step 2
  - Else → step 3

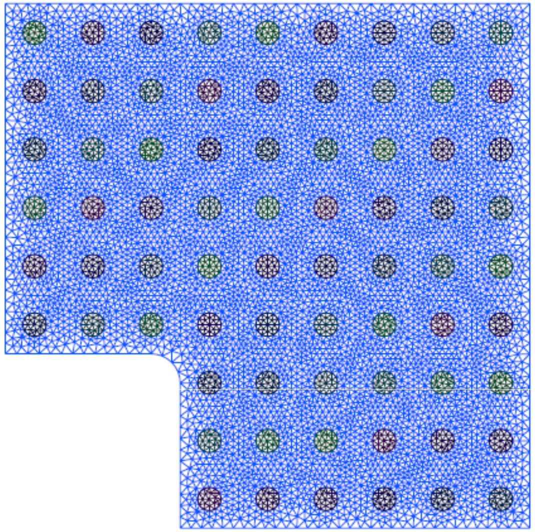
MICRO

- RVE analysis
  - Prescribe boundary condition
  - Calculate homogenized tangent operator
- RVE analysis
  - Prescribe boundary condition
  - Calculate homogenized stress
  - Calculate homogenized tangent operator

- Problem



Plane strain problem
and boundary condition



Finite element mesh

- Material
  - Matrix: $E_1 = 70GPa \quad \nu_1 = 0.3$
  - Inclusion: $E_2 = 700GPa \quad \nu_2 = 0.3$

- RVE analysis
  - Macroscopic strain

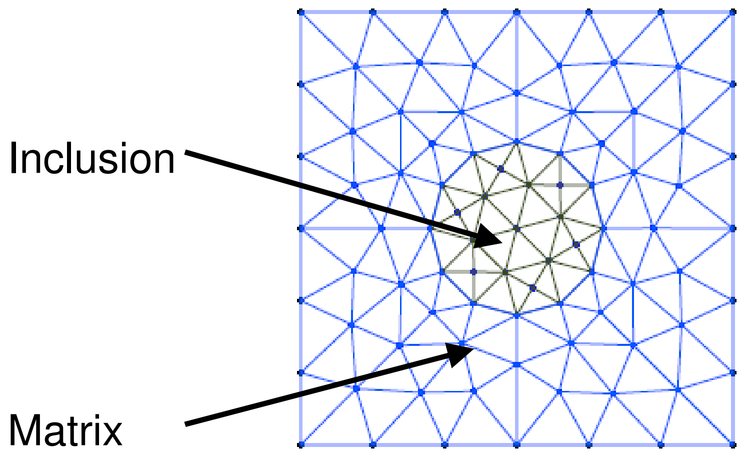
$$\bar{\varepsilon} = \begin{bmatrix} 0 & 0.05 & 0 \\ 0.05 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

  - Homogenized stress
    - Linear displacement boundary condition

$$\bar{\boldsymbol{\sigma}} = \begin{bmatrix} -0.008 & 3265.030 & 0.000 \\ 3265.030 & -0.280 & 0.000 \\ 0.000 & 0.000 & -0.086 \end{bmatrix} (MPa)$$

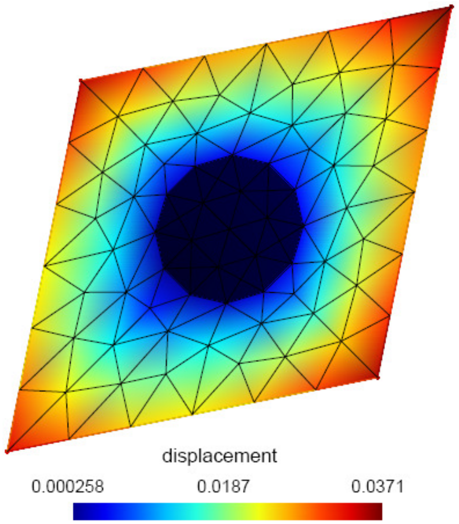
    - Periodic boundary condition

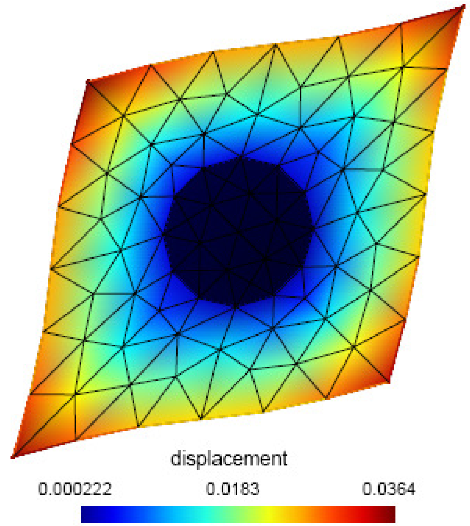
$$\bar{\boldsymbol{\sigma}} = \begin{bmatrix} 0.033 & 3177.600 & 0.000 \\ 3177.600 & -0.316 & 0.000 \\ 0.000 & 0.000 & -0.085 \end{bmatrix} (MPa)$$



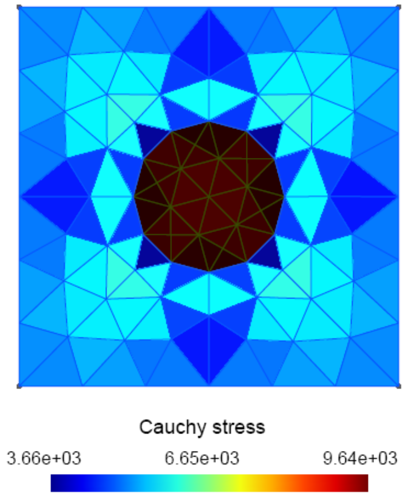
RVE finite element mesh

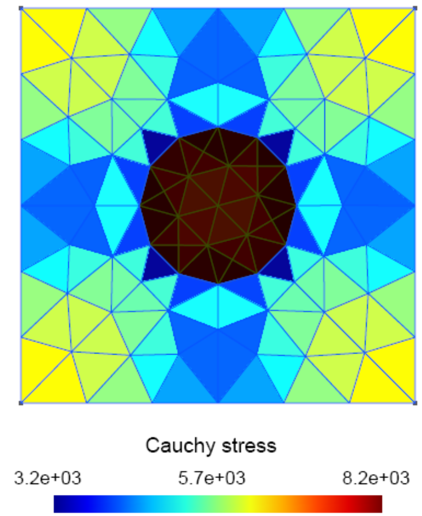
- RVE analysis
  - Displacement field





  - Von-Mises stress



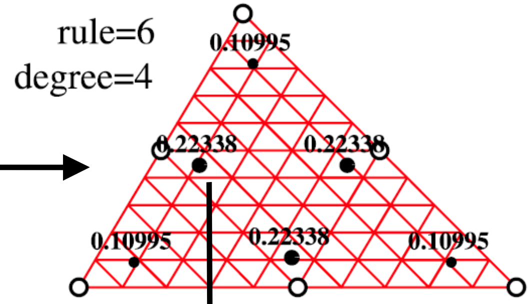


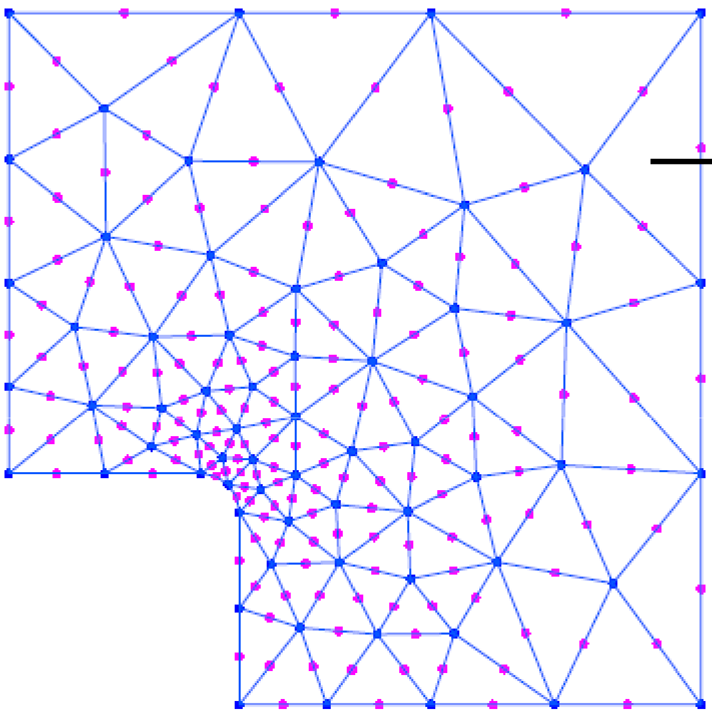
Linear displacement BC

Periodic BC

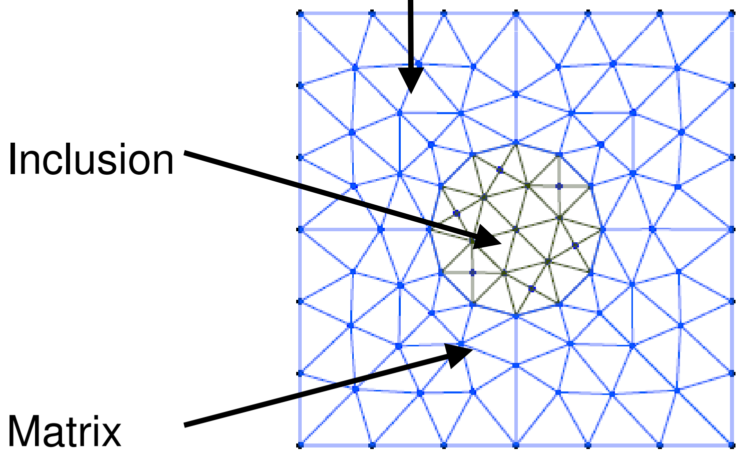
- Multi-scale analysis

Quadratic triangle





Macroscopic finite element mesh

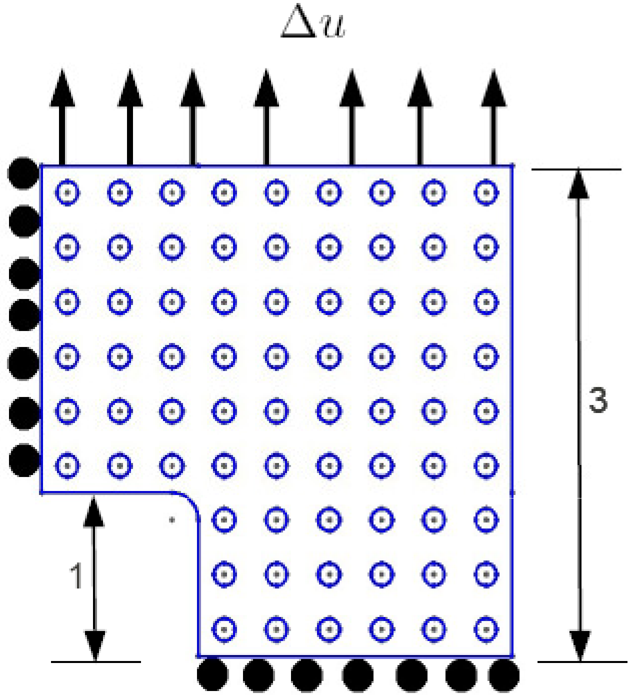


RVE finite element mesh

- Multi-scale analysis
  - Vertical displacement $\Delta u = 0.05$
  - Reaction force

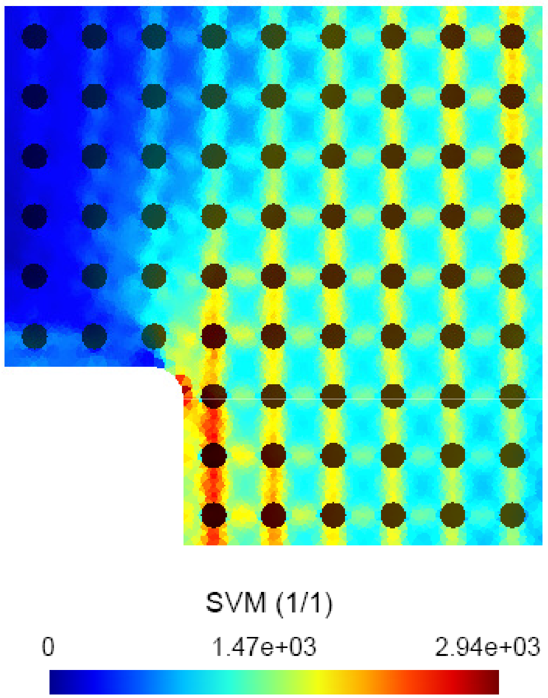
	Reaction force
Linear displacement BC	3421.955
Periodic BC	3406.800
Single scale	3381.519

Vertical displacement

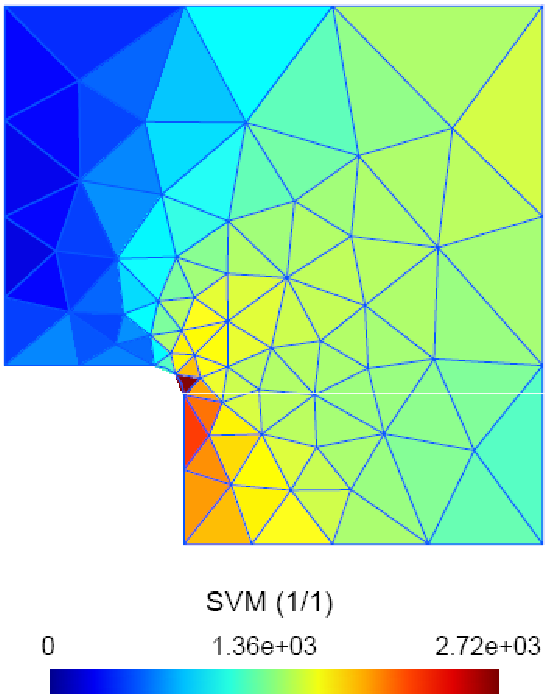


Plane strain problem and boundary condition

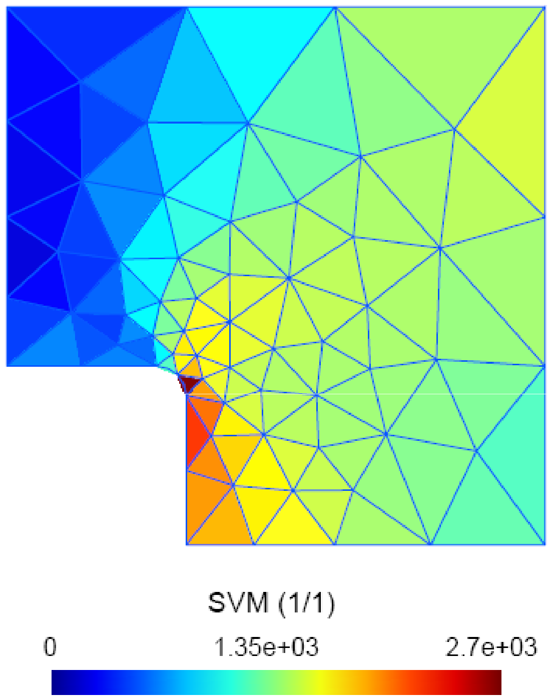
- Multi-scale analysis
  - Von-Mises stress



Single scale



Linear displacement BC



Periodic BC

Limitations

- The "scale separation" assumption sets limitations inherent to the computational multiscale method. Problems for which this assumption is invalid can not be accurately modeled using these methods.
- The computational time is still long because a microscale problem must be solved in each gauss point. Micro-problems are solved independently and parallelization can greatly reduced the computational time.
- Limitations inherent to the first-order scheme have been addressed:
  - Second-order schemes have been proposed to account for higher-order deformation gradients at the macroscale and the size effects of the RVE.
  - The continuous-discontinuous approach has been proposed to deal with problems of intense localization (e.g.: damage and fracture analysis).
  - Computational homogenization of structured thin sheets and shells, based on the application of second-order homogenization have been proposed.
  - …
- Thermo-mechanical coupling has been addressed. Coupling with other physics (heat, mechanics, electromagnetism,…) is essential to fully characterize complexe behavior of multiscale materials.

Perspectives

- Computational homogenization of emerging and evolving localization bands on the macro-scale

- Multi-physics and coupled field problems (electro-mechanical, thermo-electrical, fluid-structure interaction, magneto-electro-elasticity, acoustics, etc.)

- Dynamic problems, including inertia effects and/or propagating waves

- Problems related to non-convexity and microstructure evolution emanating from the micro-scale

- Integration of phase field models across the scales.

References

- Computational homogenization of emerging and evolving localization bands on the macro-scale
- Multi-physics and coupled field problems (electro-mechanical, thermo-electrical, fluid-structure interaction, magneto-electro-elasticity, acoustics, etc.)
- Dynamic problems, including inertia effects and/or propagating waves
- Problems related to non-convexity and microstructure evolution emanating from the micro-scale
- Integration of phase field models across the scales.

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