Unified treatment of microscopic boundary conditions in computational homogenization method for multiphysics problems

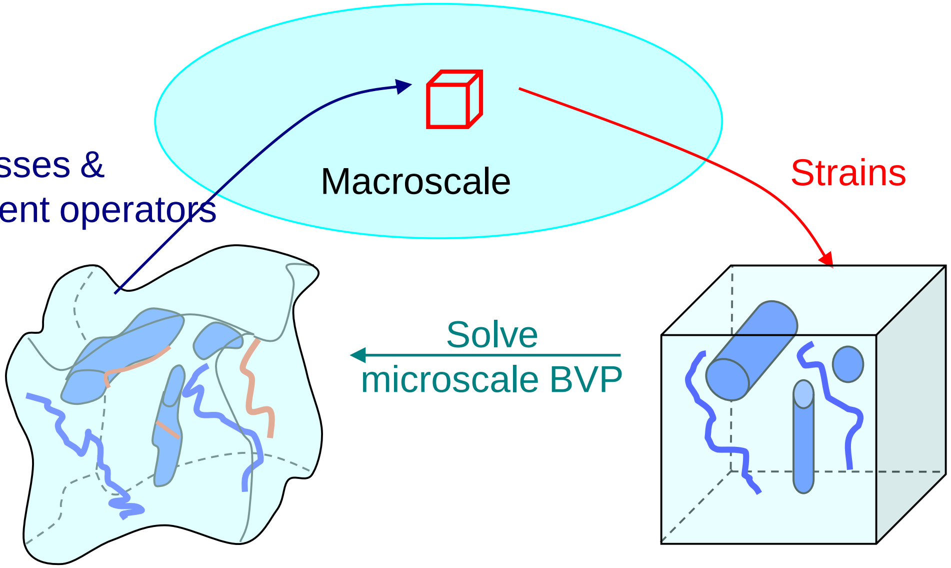
Van Dung Nguyen*, Ling Wu, Lina Homsi, Ludovic Noels

LTAS-CM3, University of Liège, Belgium

(*) vandung.nguyen@ulg.ac.be

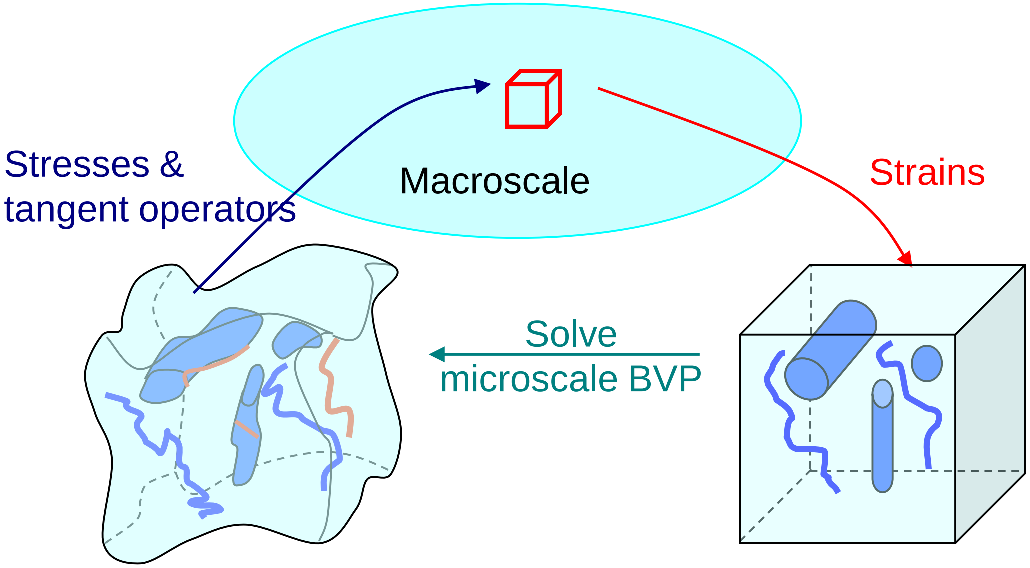
Introduction

- Computational homogenization scheme for micro-structured materials
  - Two boundary value problems (BVP) are concurrently solved
    - Macroscale BVP
    - Microscale BVP
      - Representative Volume Elements (RVE) extracted from material microstructure
      - An appropriate boundary condition
      - Constitutive laws (a priori known or can be another lower-scale BVP)
  - Separation of length scales: $L_{\text{macro}} \gg L_{\text{RVE}} \gg L_{\text{micro}}$



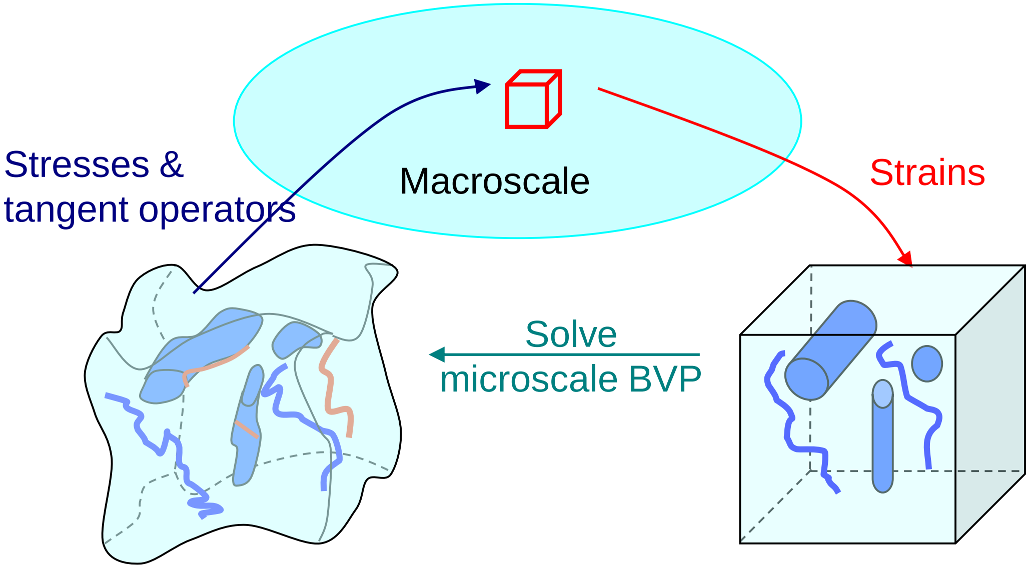
Introduction

- Computational homogenization scheme for micro-structured materials
  - Multiphysics problems can be considered
    - Mechanical (Michel et al. 1999, Feyel & Chaboche 2000, …)
    - Thermal (Ozdemir et al. 2008, Monteiro et al. 2008, …)
    - Thermo-mechanical (Ozdemir et al. 2008, Temizer et al. 2011, …)
    - Electro-mechanical (Schröder & Keip 2012, Keip et al. 2014, ...)
    - Magneto-mechanical (Javili et al. 2013, …)
    - Electro-magneto-mechanical (Schröder et al. 2015, …)
    - Etc.



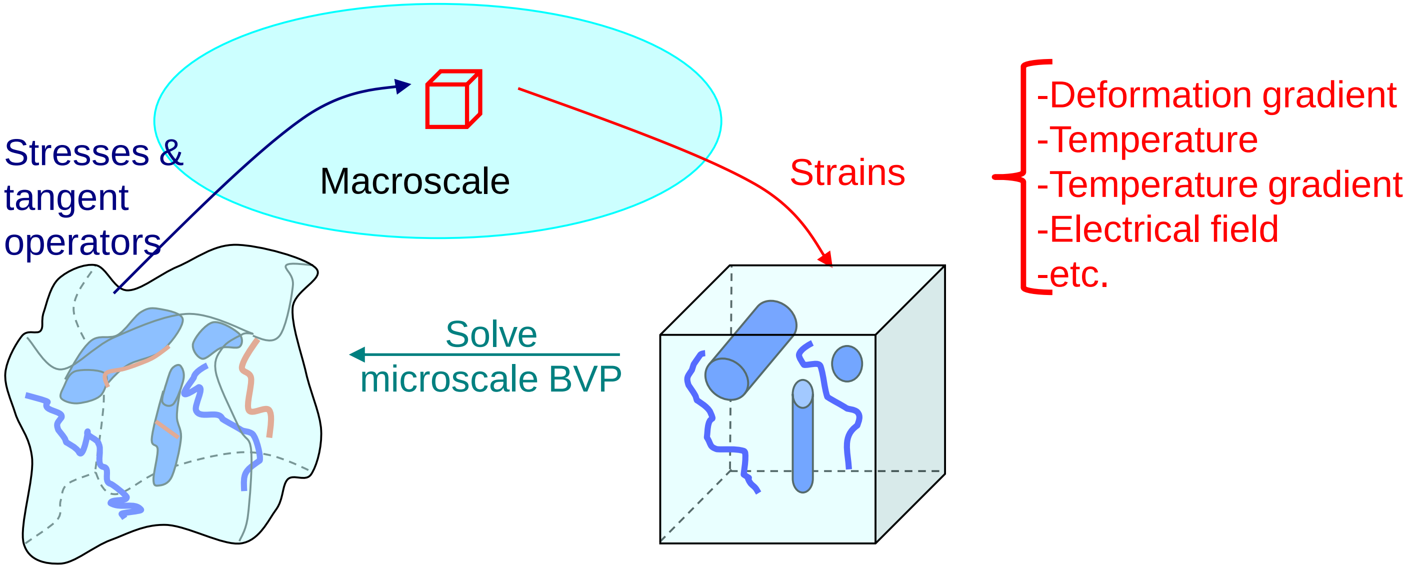
Introduction

- Computational homogenization scheme for micro-structured materials
  - Macroscale BVP
    - Formulation depending on homogenization scheme (e.g. first-order, second-order →classical Cauchy, Mindlin strain gradient)
  - Microscale BVP
    - Classical continuum mechanics for the mechanical part
    - Conventional steady balance laws for other physical phenomena (thermal, electrical, magnetic)
    - Fully-coupled constitutive laws are a priori known



Introduction

- Computational homogenization scheme for micro-structured materials
  - Macro-micro transition
    - The deformed state of the microscopic BVP is conducted by macroscopic kinematic variables
    - Macro-micro kinematic equivalence is assumed through volumetric integrals over the RVE
    - The microscopic boundary condition is given so that macro-micro transition is a priori satisfied (LDBC, PBC, MKBC, Mixed BC, etc.)



Stresses & tangent operators

Macroscale

Strains

-Deformation gradient
-Temperature
-Temperature gradient
-Electrical field
-etc.

Solve microscale BVP

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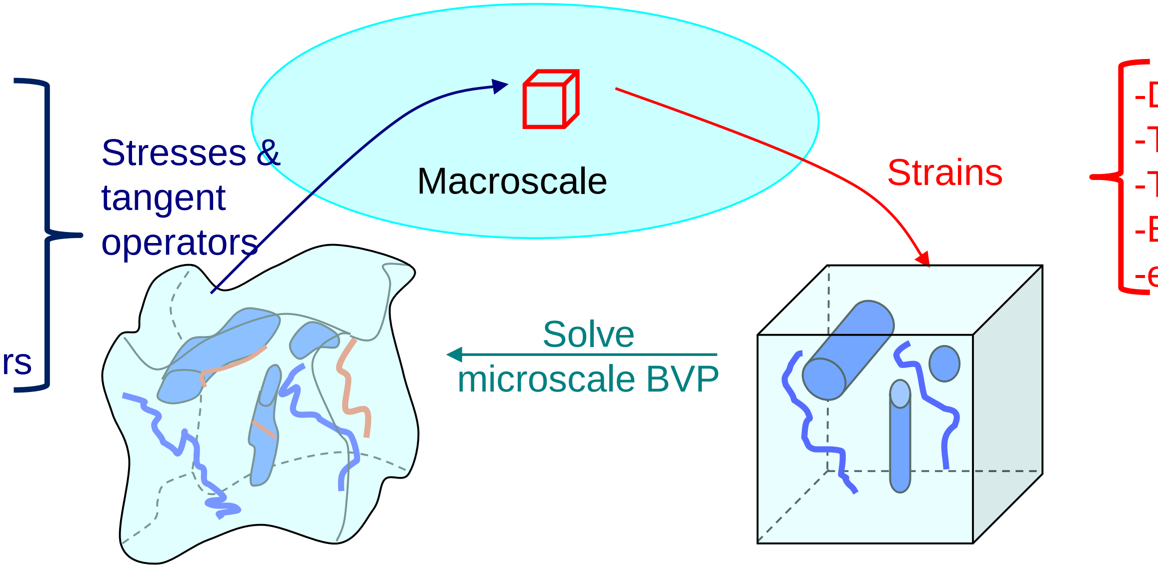
  - Micro-macro transition
    - Macroscopic stress quantities and their tangent operators are upscaled based on generalized energy equivalence statements (Hill-Mandel principle)

    → An efficient method to compute tangent operators is necessary



-First PK stress
-Thermal flux
-Heat capacity
-Electric displacement
-etc.
-related tangent operators

Stresses & tangent operators

Macroscale

Strains

Solve microscale BVP

-Deformation gradient
-Temperature
-Temperature gradient
-Electrical field
-etc.

Outline

- Microscale BVP in multiphysics
- General method to compute tangent operators
- Finite element resolution of microscale BVP
- Numerical examples
- Conclusions

Microscale BVP in multiphysics

- Strong form
  - Mechanical field $\mathbf{P}_m \cdot \boldsymbol{\nabla}_0 = \mathbf{0} \text{ on } V_0$
  - Extra-fields $\boldsymbol{\nabla}_0 \cdot \boldsymbol{\mathcal{T}}_m^k = 0 \text{ on } V_0 \text{ for } k = 1, ..., N$
  - Fully-coupled constitutive law

$$\begin{cases} \mathbf{P}_m = \mathbf{P}_m \left(\mathbf{F}_m, \theta_m^1, \boldsymbol{\varphi}_m^1, ..., \theta_m^N, \boldsymbol{\varphi}_m^N; \mathbf{Z} \right) \\ \boldsymbol{\mathcal{T}}_m^k = \boldsymbol{\mathcal{T}}_m^k \left(\mathbf{F}_m, \theta_m^1, \boldsymbol{\varphi}_m^1, ..., \theta_m^N, \boldsymbol{\varphi}_m^N; \mathbf{Z} \right) \end{cases} \quad \text{with } k = 1, ..., N$$

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- Generalized representation
  - Field

$$\boldsymbol{\mathcal{X}}_m = \left[\mathbf{x}_m^T \ \theta_m^1 \ ... \ \theta_m^N\right]^T$$

  - Field gradients

$$\boldsymbol{\mathcal{F}}_m = \left[\mathbf{F}_m^T \ \boldsymbol{\varphi}_m^1 \ ... \ \boldsymbol{\varphi}_m^N\right]^T \qquad \boldsymbol{\mathcal{F}}_m = \boldsymbol{\mathcal{X}}_m \otimes \boldsymbol{\nabla}_0$$

  - Stresses

$$\boldsymbol{\mathcal{P}}_m = \left[\mathbf{P}_m^T \ \boldsymbol{\mathcal{T}}_m^1 \ ... \ \boldsymbol{\mathcal{T}}_m^N\right]^T$$

Microscale BVP in multiphysics

- Generalized representation
  - Strong form $\boldsymbol{\mathcal{P}}_m \cdot \boldsymbol{\nabla}_0 = \mathbf{0} \text{ on } V_0$
  - Fully-coupled constitutive law $\boldsymbol{\mathcal{P}}_m = \boldsymbol{\mathcal{P}}_m \left(\boldsymbol{\mathcal{X}}_m^C, \boldsymbol{\mathcal{F}}_m ; \mathbf{Z} \right)$
    - $\boldsymbol{\mathcal{X}}_m^C$ consists of all field components appearing in the constitutive relations
    - Microscopic tangent operators

$$\boldsymbol{\mathcal{L}}_m = \frac{\partial \boldsymbol{\mathcal{P}}_m}{\partial \boldsymbol{\mathcal{F}}_m} \qquad \boldsymbol{\mathcal{J}}_m = \frac{\partial \boldsymbol{\mathcal{P}}_m}{\partial \boldsymbol{\mathcal{X}}_m^C}$$

Microscale BVP in multiphysics

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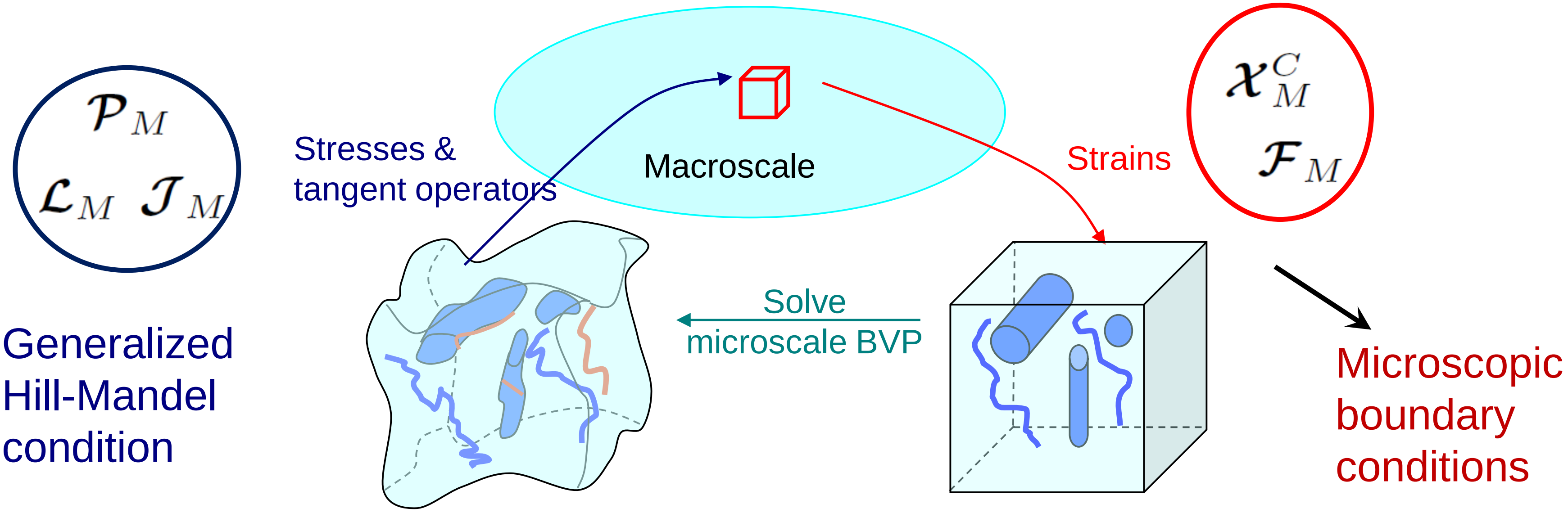
- Two-scale procedure



Generalized Hill-Mandel condition

Microscopic boundary conditions

Microscale BVP in multiphysics

- Microscopic boundary condition
  - For an arbitrary field k

$$\mathcal{X}_m^k = \Phi_m^k + \mathcal{W}_m^k \text{ on } V_0$$

Homogenous part

Fluctuation part

- First-order: $\Phi_m^k = \mathcal{X}_M^k + \boldsymbol{\mathcal{F}}_M^k \cdot \mathbf{X}_m$

  - Kinematical equivalence $\frac{1}{V_0}\int_{V_0} \boldsymbol{\mathcal{F}}_m^k \, dV = \boldsymbol{\mathcal{F}}_M^k + \frac{1}{V_0}\int_{V_0} \boldsymbol{\nabla}_0 \mathcal{W}_m^k \, dV$

$$\rightarrow \int_{\partial V_0} \mathcal{W}_m^k \mathbf{N}_m \, dS = \mathbf{0}$$

Microscale BVP in multiphysics

- Microscopic boundary condition
  - For an arbitrary field k

$$\mathcal{X}_m^k = \varPhi_m^k + \mathcal{W}_m^k \text{ on } V_0$$

Homogenous part

Fluctuation part

    - First-order: $\varPhi_m^k = \mathcal{X}_M^k + \boldsymbol{\mathcal{F}}_M^k \cdot \mathbf{X}_m$

  - Kinematical equivalence $\frac{1}{V_0}\int_{V_0} \boldsymbol{\mathcal{F}}_m^k \, dV = \boldsymbol{\mathcal{F}}_M^k + \frac{1}{V_0}\int_{V_0} \boldsymbol{\nabla}_0 \mathcal{W}_m^k \, dV$

$$\rightarrow \int_{\partial V_0} \mathcal{W}_m^k \mathbf{N}_m \, dS = \mathbf{0}$$

    - Satisfied a priori by choosing the boundary condition
      - LDBC $\mathcal{W}_m^k = 0$
      - PBC $\mathcal{W}_m^k(\mathbf{X}_m^+) = \mathcal{W}_m^k(\mathbf{X}_m^-) \ \forall \left(\mathbf{X}_m^-, \mathbf{X}_m^+\right) \in \text{ pair of facets } \left(S^i, S^{i+3}\right)$
      - Interpolation-based PBC (IPBC) $\begin{cases} \mathcal{W}_m^k\left(\mathbf{X}_m^+\right) & = \mathbb{S}^i\left(\mathbf{X}_m^-\right) \ \forall \mathbf{X}_m^+ \in S^{i+3} \\ \mathcal{W}_m^k\left(\mathbf{X}_m^-\right) & = \mathbb{S}^i\left(\mathbf{X}_m^-\right) \ \forall \mathbf{X}_m^- \in S^i \, . \end{cases}$
      - Etc.

$$\mathbb{S}^i = \sum_{k=1}^{n+1} \mathbb{N}_k^i\left(\mathbf{X}_m\right) a_k^i \ \text{(no sum on } i\text{)}$$

Microscale BVP in multiphysics

- Microscopic boundary condition
  - Field equivalence of field k

$$\frac{1}{V_0}\int_{V_0} w_m^k \, dV = w_M^k \text{ if } \mathcal{X}_m^k \text{ in } \boldsymbol{\mathcal{X}}_m^C$$

    - E.g. temperature field with the capacity equivalence

$$\begin{cases} w_m^k = C_m^k \mathcal{X}_m^k \\ w_M^k = C_M^k \mathcal{X}_M^k \end{cases}$$

$$C_M^k = \frac{1}{V_0}\int_{V_0} C_m^k \, dV$$

Microscale BVP in multiphysics

- Micro-macro transition
  - Based on the generalized Hill-Mandel principle
  - Homogenized stresses

$$\boldsymbol{\mathcal{P}}_M = \frac{1}{V_0}\int_{V_0} \boldsymbol{\mathcal{P}}_m \, dV$$

  - Quantities other than homogenized stresses (thermo-elastic heating, damage …)

$$\boldsymbol{\mathcal{Z}}_M = \frac{1}{V_0}\int_{V_0} \boldsymbol{\mathcal{Z}}_m \, dV$$

  - Homogenized tangent operators

$$\boldsymbol{\mathcal{L}}_M = \frac{\partial \boldsymbol{\mathcal{P}}_M}{\partial \boldsymbol{\mathcal{F}}_M} \qquad \boldsymbol{\mathcal{J}}_M = \frac{\partial \boldsymbol{\mathcal{P}}_M}{\partial \boldsymbol{\mathcal{X}}_M^C}$$

$$\boldsymbol{\mathcal{Y}}_{\boldsymbol{\mathcal{F}}_M} = \frac{\partial \boldsymbol{\mathcal{Z}}_M}{\partial \boldsymbol{\mathcal{F}}_M} \qquad \boldsymbol{\mathcal{Y}}_{\boldsymbol{\mathcal{X}}_M^C} = \frac{\partial \boldsymbol{\mathcal{Z}}_M}{\partial \boldsymbol{\mathcal{X}}_M^C}$$

→This work provides an efficient method to compute these tangent operators

General method to compute tangent operators

- Homogenized tangent operator is estimated at the converged solution
  - Homogenized stresses

$$\begin{bmatrix} \boldsymbol{\mathcal{P}}_M \\ \boldsymbol{\mathcal{Z}}_M \end{bmatrix} = \frac{1}{V_0} \sum_e \int_{V_0^e} \begin{bmatrix} \boldsymbol{\mathcal{P}}_m \\ \boldsymbol{\mathcal{Z}}_m \end{bmatrix} dV$$

  - Homogenized tangent operators

$$\begin{bmatrix} \boldsymbol{\mathcal{L}}_M & \boldsymbol{\mathcal{J}}_M \\ \boldsymbol{\mathcal{Y}}_{\boldsymbol{\mathcal{F}}_M} & \boldsymbol{\mathcal{Y}}_{\boldsymbol{\mathcal{X}}_M^C} \end{bmatrix} = \begin{bmatrix} \frac{\partial \boldsymbol{\mathcal{P}}_M}{\partial \boldsymbol{\mathcal{K}}_M} \\ \frac{\partial \boldsymbol{\mathcal{Z}}_M}{\partial \boldsymbol{\mathcal{K}}_M} \end{bmatrix} = \frac{1}{V_0} \sum_e \int_{V_0^e} \begin{bmatrix} \boldsymbol{\mathcal{L}}_m \mathbf{B}^e & \boldsymbol{\mathcal{J}}_m \mathbf{N}^e \\ \boldsymbol{\mathcal{Y}}_{\boldsymbol{\mathcal{F}}_m} \mathbf{B}^e & \boldsymbol{\mathcal{Y}}_{\boldsymbol{\mathcal{X}}_m^C} \mathbf{N}^e \end{bmatrix} dV \frac{\partial \left[\boldsymbol{\mathcal{U}}\right]_{V_0^e}}{\partial \boldsymbol{\mathcal{K}}_M}$$

$$\boldsymbol{\mathcal{K}}_M = \begin{bmatrix} \boldsymbol{\mathcal{F}}_M \\ \boldsymbol{\mathcal{X}}_M^C \end{bmatrix}$$ macroscopic kinematic variable applied to the microscale BVP

$$[\boldsymbol{\mathcal{U}}]_{V_0^e}$$ microscopic unknowns of element e

General method to compute tangent operators

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  - Homogenized tangent operators

$$\begin{bmatrix}\mathcal{L}_M & \mathcal{J}_M\\ \mathcal{Y}_{\mathcal{F}_M} & \mathcal{Y}_{\mathcal{X}^C_M}\end{bmatrix} = \begin{bmatrix}\frac{\partial \mathcal{P}_M}{\partial \mathcal{K}_M}\\ \frac{\partial \mathcal{Z}_M}{\partial \mathcal{K}_M}\end{bmatrix} = \frac{1}{V_0}\sum_e \int_{V_0^e} \begin{bmatrix}\mathcal{L}_m\mathbf{B}^e & \mathcal{J}_m\mathbf{N}^e\\ \mathcal{Y}_{\mathcal{F}_m}\mathbf{B}^e & \mathcal{Y}_{\mathcal{X}^C_m}\mathbf{N}^e\end{bmatrix} dV \frac{\partial \left[\mathcal{U}\right]_{V_0^e}}{\partial \mathcal{K}_M}$$

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$[\mathcal{U}]_{V_0^e}$ microscopic unknowns of element e

  - After assembling

$$\begin{bmatrix}\mathcal{L}_M & \mathcal{J}_M\\ \mathcal{Y}_{\mathcal{F}_M} & \mathcal{Y}_{\mathcal{X}^C_M}\end{bmatrix} = \mathbf{D}\frac{\partial \mathcal{U}}{\partial \mathcal{K}_M}$$

$\mathcal{U}$ microscopic unknowns

    - Matrix **D** can be easily estimated

$$\mathbf{D} = \bigwedge_{\mathbf{V_0^e}\in\mathbf{V_0}} \left(\frac{1}{V_0}\int_{V_0^e} \begin{bmatrix}\mathcal{L}_m\mathbf{B}^e & \mathcal{J}_m\mathbf{N}^e\\ \mathcal{Y}_{\mathcal{F}_m}\mathbf{B}^e & \mathcal{Y}_{\mathcal{X}^C_m}\mathbf{N}^e\end{bmatrix} dV\right)$$

Need to estimate:

$$\frac{\partial \mathcal{U}}{\partial \mathcal{K}_M}$$

Finite element resolution of microscale BVP

- Microscopic boundary condition in FE discretization

$$\mathbf{C}\boldsymbol{\mathcal{U}} - \mathbf{S}\boldsymbol{\mathcal{K}}_M = 0$$

$$\boldsymbol{\mathcal{K}}_M = \begin{bmatrix} \boldsymbol{\mathcal{F}}_M \\ \boldsymbol{\mathcal{X}}_M^C \end{bmatrix}$$ macroscopic kinematic variable applied to the microscale BVP

$\boldsymbol{\mathcal{U}}$ microscopic unknowns

  - Constraint matrices (**C** and **S**) depend on the BC type (LDBC, PBC, IPBC, MKBC, etc.)

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  - Constraint matrices (**C** and **S**) depend on the BC type (LDBC, PBC, IPBC, MKBC, etc.)

- Microscopic equilibrium equations with Lagrange multipliers

$$\begin{cases} \mathbf{f}_m\left(\mathcal{U}\right) - \mathbf{C}^T\boldsymbol{\lambda} = \mathbf{0} \\ \mathbf{C}\mathcal{U} - \mathbf{S}\mathcal{K}_M = \mathbf{0} \end{cases}$$

  - Multiplier elimination

$$\begin{cases} \mathbf{r} = \mathbf{f}_m - \mathbf{C}^T\boldsymbol{\lambda} = \mathbf{Q}^T\mathbf{f}_m = \mathbf{0} \\ \mathbf{r}_c = \mathbf{C}\mathcal{U} - \mathbf{S}\mathcal{K}_M = \mathbf{0} \end{cases}$$

$$\boldsymbol{\lambda} = \mathbf{R}^T\mathbf{f}_m$$

$$\mathbf{R}^T = \left(\mathbf{C}\mathbf{C}^T\right)^{-1}\mathbf{C}$$

$$\mathbf{Q} = \mathbf{I} - \mathbf{R}\mathbf{C}$$

    - Considering $\mathcal{U}$ as unknowns only
    - Need to estimate $\frac{\partial \mathcal{U}}{\partial \mathcal{K}_M}$ for tangent estimation

Finite element resolution of microscale BVP

- Microscopic equilibrium equations with Lagrange multipliers

$$\begin{cases} \mathbf{r} = \mathbf{f}_m - \mathbf{C}^T \boldsymbol{\lambda} = \mathbf{Q}^T \mathbf{f}_m = \mathbf{0} \\ \mathbf{r}_c = \mathbf{C}\mathcal{U} - \mathbf{S}\mathcal{K}_M = \mathbf{0} \end{cases}$$

  - Linearized system

$$\begin{cases} \mathbf{r} + \mathbf{Q}^T \mathbf{K} \Delta\mathcal{U} = \mathbf{0} \\ \mathbf{r}_c + \mathbf{C}\Delta\mathcal{U} - \mathbf{S}\delta\mathcal{K}_M = \mathbf{0} \end{cases} \Longrightarrow \begin{cases} \mathbf{Q}^T \mathbf{K} \mathbf{Q} \Delta\mathcal{U} + \mathbf{r} - \mathbf{V}\left(\mathbf{r}_c - \mathbf{S}\delta\mathcal{K}_M\right) = \mathbf{0} \\ \mathbf{C}\Delta\mathcal{U} + \mathbf{r}_c - \mathbf{S}\delta\mathcal{K}_M = \mathbf{0} \end{cases}$$

$$\mathbf{V} = \mathbf{Q}^T \mathbf{K} \mathbf{R}$$

  - $\mathcal{U}$ can be obtained by considering $\delta\mathcal{K}_M = \mathbf{0}$
    - Iterative loop

$$\Delta\mathcal{U} = -\tilde{\mathbf{K}}^{-1} \tilde{\mathbf{r}}$$

$$\mathcal{U} = \mathcal{U} + \Delta\mathcal{U}$$

until $\dfrac{\| \tilde{\mathbf{r}} \|}{\| \mathbf{f}_m \|} < \epsilon$

$$\tilde{\mathbf{K}} = \mathbf{C}^T \mathbf{C} + \mathbf{Q}^T \mathbf{K} \mathbf{Q} \,,$$

$$\tilde{\mathbf{r}} = \mathbf{r} + \left(\mathbf{C}^T - \mathbf{V}\right) \mathbf{r}_c$$

(Ainsworth 2001)

Finite element resolution of microscale BVP

- Microscopic equilibrium equations with Lagrange multipliers

$$\begin{cases} \mathbf{r} = \mathbf{f}_m - \mathbf{C}^T \boldsymbol{\lambda} = \mathbf{Q}^T \mathbf{f}_m = \mathbf{0} \\ \mathbf{r}_c = \mathbf{C}\boldsymbol{\mathcal{U}} - \mathbf{S}\boldsymbol{\mathcal{K}}_M = \mathbf{0} \end{cases}$$

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$$\mathbf{V} = \mathbf{Q}^T \mathbf{K} \mathbf{R}$$

  - $\dfrac{\partial \boldsymbol{\mathcal{U}}}{\partial \boldsymbol{\mathcal{K}}_M}$ can be obtained by considering the linearized system at the converged solution

$$\begin{cases} \mathbf{Q}^T \mathbf{K} \mathbf{Q} \delta\boldsymbol{\mathcal{U}} + \mathbf{V}\mathbf{S}\delta\boldsymbol{\mathcal{K}}_M = \mathbf{0} \\ \mathbf{C}\delta\boldsymbol{\mathcal{U}} - \mathbf{S}\delta\boldsymbol{\mathcal{K}}_M = \mathbf{0} \end{cases} \Longrightarrow \frac{\partial \boldsymbol{\mathcal{U}}}{\partial \boldsymbol{\mathcal{K}}_M} = \left(\tilde{\mathbf{K}}\right)^{-1} \mathbf{Y}$$

    - Multiple right hand side system $\mathbf{Y} = \left(\mathbf{C}^T - \mathbf{V}\right)\mathbf{S}$
    - Obtained by using the microscopic stiffness matrix $\tilde{\mathbf{K}} = \mathbf{C}^T \mathbf{C} + \mathbf{Q}^T \mathbf{K} \mathbf{Q}$

Finite element resolution of microscale BVP

- Microscopic equilibrium equations with Lagrange multipliers

$$\begin{cases} \mathbf{r} = \mathbf{f}_m - \mathbf{C}^T \boldsymbol{\lambda} = \mathbf{Q}^T \mathbf{f}_m = \mathbf{0} \\ \mathbf{r}_c = \mathbf{C}\boldsymbol{\mathcal{U}} - \mathbf{S}\boldsymbol{\mathcal{K}}_M = \mathbf{0} \end{cases}$$

  - Linearized system

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$$\mathbf{V} = \mathbf{Q}^T \mathbf{K} \mathbf{R}$$

  - $\dfrac{\partial \boldsymbol{\mathcal{U}}}{\partial \boldsymbol{\mathcal{K}}_M}$ can be obtained by considering the linearized system at the converged solution

$$\begin{cases} \mathbf{Q}^T \mathbf{K} \mathbf{Q} \delta\boldsymbol{\mathcal{U}} + \mathbf{V}\mathbf{S}\delta\boldsymbol{\mathcal{K}}_M = \mathbf{0} \\ \mathbf{C}\delta\boldsymbol{\mathcal{U}} - \mathbf{S}\delta\boldsymbol{\mathcal{K}}_M = \mathbf{0} \end{cases} \Longrightarrow \frac{\partial \boldsymbol{\mathcal{U}}}{\partial \boldsymbol{\mathcal{K}}_M} = \left(\tilde{\mathbf{K}}\right)^{-1} \mathbf{Y}$$

    - Multiple right hand side system $\mathbf{Y} = \left(\mathbf{C}^T - \mathbf{V}\right)\mathbf{S}$
    - Obtained by using the microscopic stiffness matrix $\tilde{\mathbf{K}} = \mathbf{C}^T\mathbf{C} + \mathbf{Q}^T \mathbf{K} \mathbf{Q}$

If the direct solver (e.g. LU) is used to solve the microscale BVP, matrix $\tilde{\mathbf{K}}$ is already factorized. This multiple RHS system then reconsiders this factorized matrix → computational time is largely reduced

Finite element resolution of microscale BVP

- Microscopic boundary condition in FE discretization

$$\mathbf{C}\mathcal{U} - \mathbf{S}\mathcal{K}_M = 0$$

$$\mathcal{K}_M = \begin{bmatrix}\mathcal{F}_M \\ \mathcal{X}_M^C\end{bmatrix}$$ macroscopic kinematic variable applied to the microscale BVP

$$\mathcal{U}$$ microscopic unknowns

  - Constraint matrices (**C** and **S**) depend on the BC type (LDBC, PBC, IPBC, MKBC, etc.)

- Microscopic equilibrium equations with constraint elimination method
  - Total unknowns is decomposed into
    - Internal part $\mathcal{U}_i$
    - Dependent part $\mathcal{U}_d$
    - Independent part $\mathcal{U}_f$
    - Direct constraint part $\mathcal{U}_c$

$$\begin{cases}\mathbf{C}_d\mathcal{U}_d + \mathbf{C}_f\mathcal{U}_f + \mathbf{C}_c\mathcal{U}_c = \mathbf{S}_d\mathcal{K}_M \\ \mathcal{U}_c = \mathbf{S}_c\mathcal{K}_M\end{cases}$$

$$\begin{cases}\mathcal{U}_d = \mathbf{C}_{df}\mathcal{U}_f + \mathbf{S}_{df}\mathcal{K}_M \\ \mathcal{U}_c = \mathbf{S}_c\mathcal{K}_M\end{cases}$$

  - True unknowns $\tilde{\mathcal{U}} = \left[\mathcal{U}_i^T \ \mathcal{U}_f^T\right]^T$

$$\mathcal{U} = \begin{bmatrix}\mathcal{U}_i \\ \mathcal{U}_d \\ \mathcal{U}_f \\ \mathcal{U}_c\end{bmatrix} = \mathbf{T}\tilde{\mathcal{U}} + \tilde{\mathbf{S}}\mathcal{K}_M$$

$$\mathbf{T} = \begin{bmatrix}\mathbf{I}_{n_i} & \mathbf{0}_{n_i \times n_f} \\ \mathbf{0}_{n_d \times n_i} & \mathbf{C}_{df} \\ \mathbf{0}_{n_f \times n_i} & \mathbf{I}_{n_f} \\ \mathbf{0}_{n_c \times n_i} & \mathbf{0}_{n_c \times n_f}\end{bmatrix} \quad \tilde{\mathbf{S}} = \begin{bmatrix}\mathbf{0}_{n_i \times (3+N)} \\ \mathbf{S}_{df} \\ \mathbf{0}_{n_f \times (3+N)} \\ \mathbf{S}_c\end{bmatrix}$$

Finite element resolution of microscale BVP

- We can have a similar result with the constraint elimination method

$$\mathbf{T}^T \mathbf{f}_m = \mathbf{0}$$

$$\mathcal{U} = \mathbf{T}\tilde{\mathcal{U}} + \tilde{\mathbf{S}}\mathcal{K}_M$$

  - $\frac{\partial \mathcal{U}}{\partial \mathcal{K}_M}$ can be obtained by considering the linearized system at the converged solution

$$\mathbf{T}^T \mathbf{K} \delta\mathcal{U} = \mathbf{0}$$

$$\delta\mathcal{U} = \mathbf{T}\delta\tilde{\mathcal{U}} + \tilde{\mathbf{S}}\delta\mathcal{K}_M$$

$$\Rightarrow \quad \tilde{\mathbf{K}}\delta\tilde{\mathcal{U}} = -\mathbf{Z}\delta\mathcal{K}_M \quad \Rightarrow \quad \frac{\partial \mathcal{U}}{\partial \mathcal{K}_M} = \tilde{\mathbf{S}} - \mathbf{T}\tilde{\mathbf{K}}^{-1}\mathbf{Z}$$

  - Multiple right hand side system $\mathbf{Z} = \mathbf{T}^T \mathbf{K}\tilde{\mathbf{S}}$
  - Obtained by using the microscopic stiffness matrix $\tilde{\mathbf{K}} = \mathbf{T}^T \mathbf{K}\mathbf{T}$

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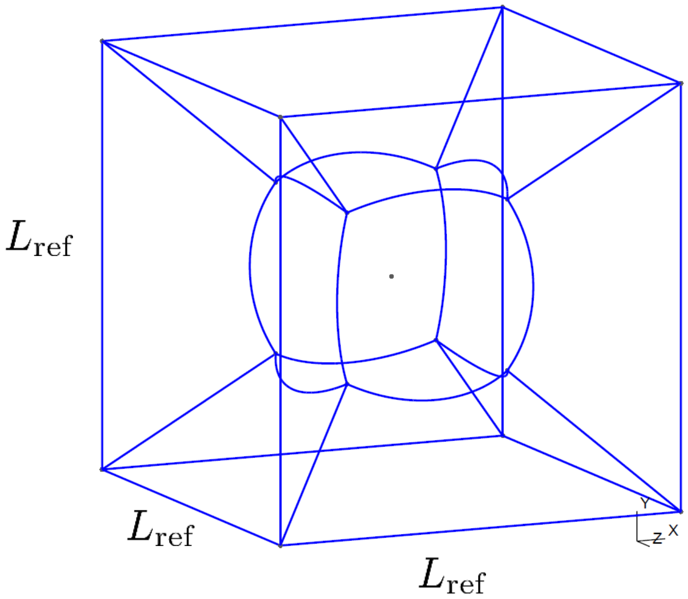
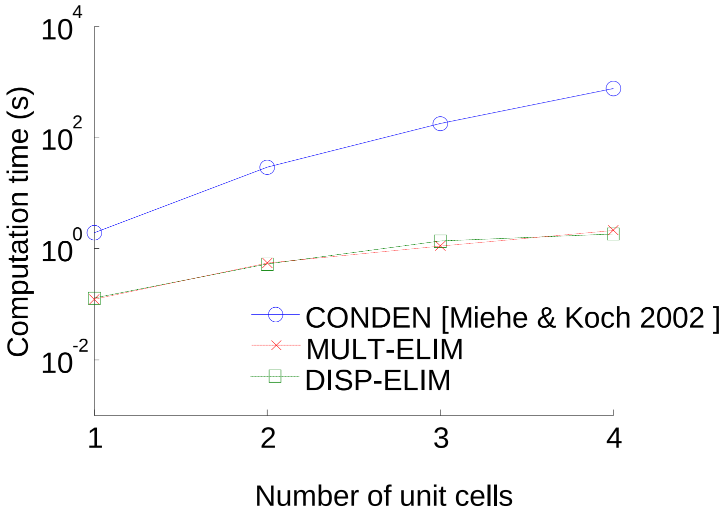
If the direct solver (e.g. LU) is used to solve the microscale BVP, matrix $\tilde{\mathbf{K}}$ is already factorized. This multiple RHS system then reconsiders this factorized matrix → computational time is largely reduced

Numerical examples

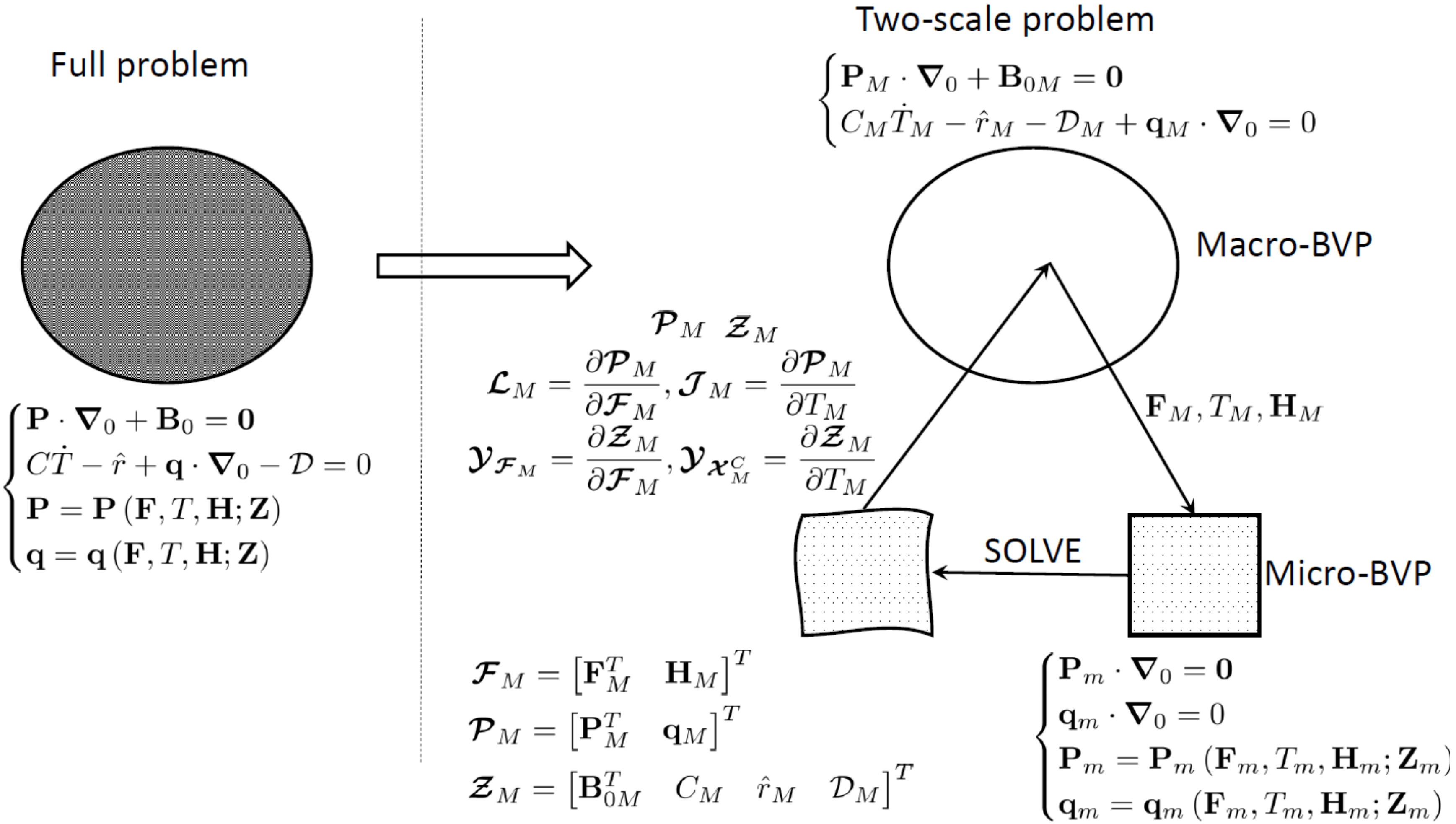
- Computation efficiency
  - Linear elastic material
  - A unit cell consisting of a spherical void of radius $0.2L_{\mathrm{ref}}$
  - RVE dimensions ranging from $L_{\mathrm{ref}} \times L_{\mathrm{ref}} \times L_{\mathrm{ref}}$ to $4L_{\mathrm{ref}} \times 4L_{\mathrm{ref}} \times L_{\mathrm{ref}}$





Numerical examples

- Fully-coupled thermo-elastoplastic problem



Full problem

$$\begin{cases} \mathbf{P} \cdot \boldsymbol{\nabla}_0 + \mathbf{B}_0 = \mathbf{0} \\ C\dot{T} - \hat{r} + \mathbf{q} \cdot \boldsymbol{\nabla}_0 - \mathcal{D} = 0 \\ \mathbf{P} = \mathbf{P}\left(\mathbf{F}, T, \mathbf{H}; \mathbf{Z}\right) \\ \mathbf{q} = \mathbf{q}\left(\mathbf{F}, T, \mathbf{H}; \mathbf{Z}\right) \end{cases}$$

Two-scale problem

$$\begin{cases} \mathbf{P}_M \cdot \boldsymbol{\nabla}_0 + \mathbf{B}_{0M} = \mathbf{0} \\ C_M \dot{T}_M - \hat{r}_M - \mathcal{D}_M + \mathbf{q}_M \cdot \boldsymbol{\nabla}_0 = 0 \end{cases}$$

$\boldsymbol{\mathcal{P}}_M \quad \boldsymbol{\mathcal{Z}}_M$

$$\boldsymbol{\mathcal{L}}_M = \frac{\partial \boldsymbol{\mathcal{P}}_M}{\partial \boldsymbol{\mathcal{F}}_M}, \boldsymbol{\mathcal{J}}_M = \frac{\partial \boldsymbol{\mathcal{P}}_M}{\partial T_M}$$

$$\boldsymbol{\mathcal{Y}}_{\boldsymbol{\mathcal{F}}_M} = \frac{\partial \boldsymbol{\mathcal{Z}}_M}{\partial \boldsymbol{\mathcal{F}}_M}, \boldsymbol{\mathcal{Y}}_{\boldsymbol{\mathcal{X}}^C_M} = \frac{\partial \boldsymbol{\mathcal{Z}}_M}{\partial T_M}$$

$\mathbf{F}_M, T_M, \mathbf{H}_M$

$$\boldsymbol{\mathcal{F}}_M = \begin{bmatrix} \mathbf{F}_M^T & \mathbf{H}_M \end{bmatrix}^T$$

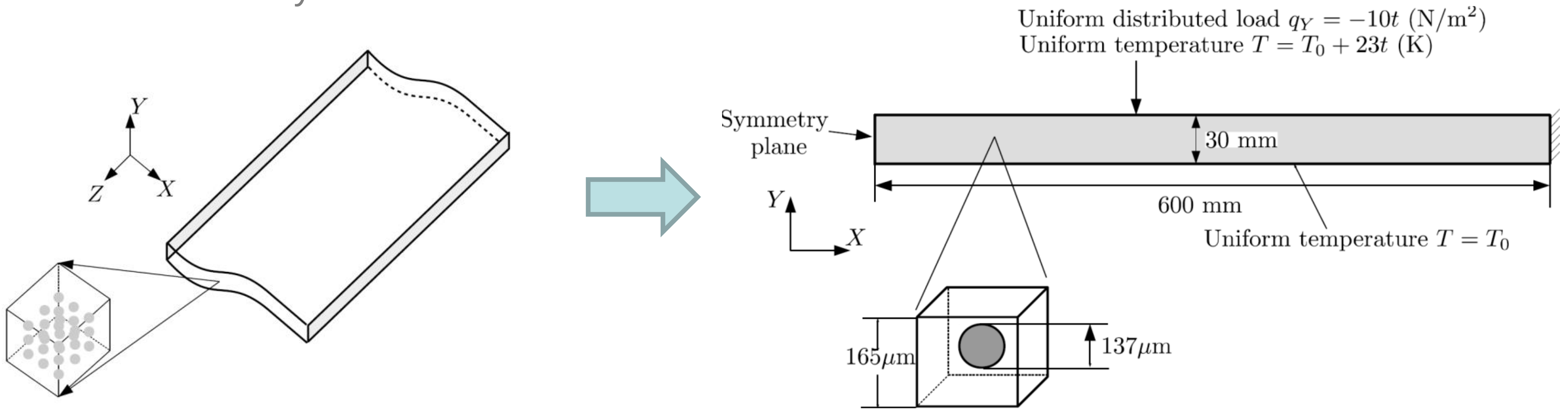
$$\boldsymbol{\mathcal{P}}_M = \begin{bmatrix} \mathbf{P}_M^T & \mathbf{q}_M \end{bmatrix}^T$$

$$\boldsymbol{\mathcal{Z}}_M = \begin{bmatrix} \mathbf{B}_{0M}^T & C_M & \hat{r}_M & \mathcal{D}_M \end{bmatrix}^T$$

$$\begin{cases} \mathbf{P}_m \cdot \boldsymbol{\nabla}_0 = \mathbf{0} \\ \mathbf{q}_m \cdot \boldsymbol{\nabla}_0 = 0 \\ \mathbf{P}_m = \mathbf{P}_m\left(\mathbf{F}_m, T_m, \mathbf{H}_m; \mathbf{Z}_m\right) \\ \mathbf{q}_m = \mathbf{q}_m\left(\mathbf{F}_m, T_m, \mathbf{H}_m; \mathbf{Z}_m\right) \end{cases}$$

Numerical examples

- Fully-coupled thermo-elastoplastic problem
  - Geometry



  - Fully-coupled thermo-elastoplastic law

Constant	Notation (unit)	Matrix	Fiber
Bulk modulus	K (GPa)	73.53	213.89
Shear modulus	μ (GPa)	28.19	160.42
Initial yield stress	τ_{y0} (MPa)	300	
Hardening modulus	H_0 (MPa)	150	
Thermal expansion coefficient	α (10^{-6}K^{-1})	23.6	5
Thermal conductivity	κ (Wm^{-1}K^{-1})	247	38
Specific heat capacity	C (10^6 Jm^{-3}K^{-1})	2.43	3.38

(Ozdemir et al. 2008)

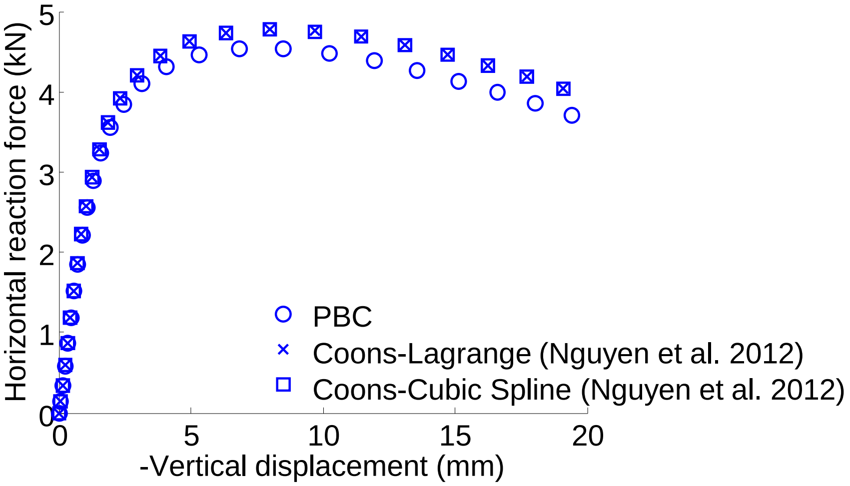
- Thermal softening ($\omega_T = 0.002K^{-1}$)

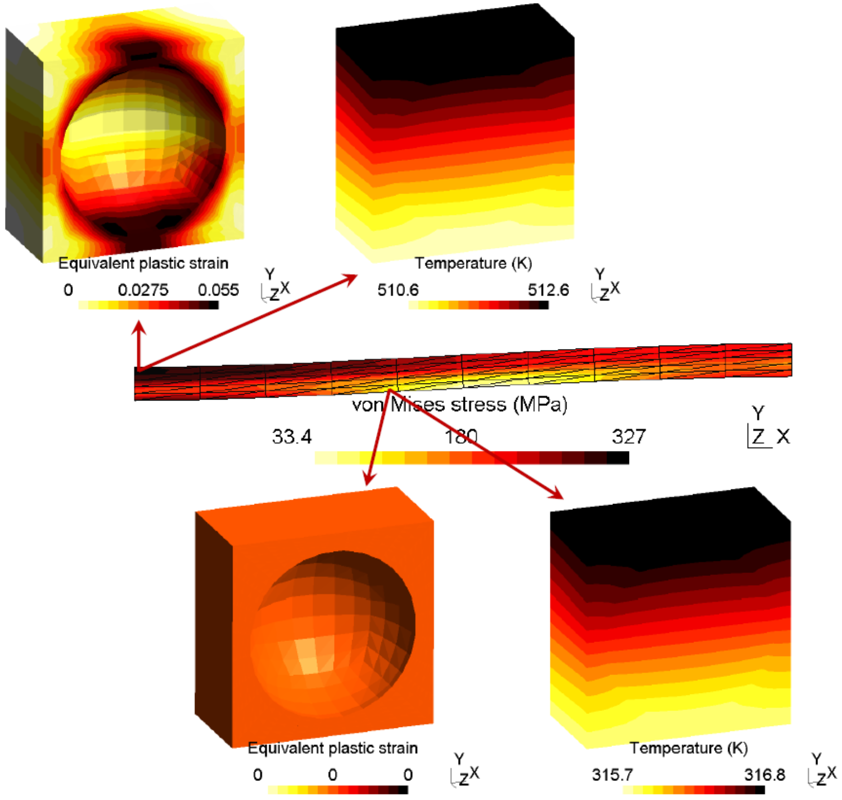
$$\tau_y(\gamma, T_m) = (\tau_{y0} + H_0\gamma)\left[1 - \omega_T (T_m - T_0)\right]$$

- Mechanical heating characterized by the Taylor-Quinney factor $\beta = 0.9$

Numerical examples

- Fully-coupled thermo-elastoplastic problem





Conclusions

- An arbitrary kind of microscopic boundary condition can be applied in multi-scale computational homogenization analyses

- The macroscopic tangent operators can be directly estimated without any significant computational cost

- The capability of the proposed procedure is demonstrated in the microscopic analyses as well as in a fully-coupled thermo-mechanical two-scale problem

Thank you for your attention !