Alternative numerical method in continuum mechanics

COMPUTATIONAL MULTISCALE

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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.
Why use computational multiscale methods?

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 successfully 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.
CMM – Basic assumptions

- Material macroscopically sufficiently homogeneous, but microscopically heterogeneous (inclusions, grains, interfaces, cavities,...) \( \rightarrow \) (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).

\[
\begin{align*}
l_a & \ll l_d \ll l_m \ll l_M \\
\end{align*}
\]

Heterogeneous micro-structure associated with macroscopic continuum point M
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

- Macroscopic problem

\[ \nabla \cdot \bar{\sigma}^T + \bar{b} = 0 \]

\[ \int_{\bar{B}} \bar{\sigma} : \nabla \delta \varphi \, dV = \int_{\partial_N \bar{B}} \bar{T} : \nabla \delta \varphi \, dS + \int_{\bar{B}} \bar{b} : \nabla \delta \varphi \, dV \]
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.

• Selection of RVE
  – RVE contains all necessary information of micro-structure
  – Computation efficiency

• RVE equilibrium state
  – In absence of body forces: \( \nabla \cdot \sigma^T = 0 \)
  – Constitutive law: \( \sigma^{(i)} = F_i(\varepsilon) \)
    – For hyper-elastic material \( \sigma = \partial_\varepsilon W \)
  – Equilibrium state of the RVE is assumed to be consistent with the boundary condition, which are related to the macroscopic strain field
Definition of microscopic problem

- **Boundary condition**
  - Strain driven problem
  - Microscopic strain: \[ \varepsilon = \frac{1}{2} (\nabla \otimes \mathbf{u} + \mathbf{u} \otimes \nabla) = \nabla \otimes_s \mathbf{u} \]
  - Macroscopic strain:
    \[ \bar{\varepsilon} = \frac{1}{V} \int_V \varepsilon \, dV \]
  - Using Gauss theorem:
    \[ \bar{\varepsilon} = \frac{1}{V} \oint_{\partial V} \mathbf{n} \otimes_s \mathbf{u} \, dS \]
    \[ \frac{1}{V} \oint_{\partial V} \mathbf{n} \otimes_s (\mathbf{u} - \bar{\varepsilon} \mathbf{x}) \, dS = 0 \]
  - Split of displacement field: mean part and fluctuation part:
    \[ \mathbf{u} = \bar{\mathbf{u}} + \tilde{\mathbf{u}} = \bar{\varepsilon} \mathbf{x} + \tilde{\mathbf{u}} \quad \varepsilon = \bar{\varepsilon} + \nabla \otimes_s \tilde{\mathbf{u}} \quad \varepsilon = \bar{\varepsilon} + \tilde{\varepsilon} \]
  - Constrain on the fluctuation field:
    \[ \frac{1}{V} \oint_{\partial V} \mathbf{n} \otimes_s \tilde{\mathbf{u}} \, dS = 0 \quad (*) \]
  - Boundary condition must be defined to satisfy (*).
Definition of microscopic problem

- **Boundary condition**
  - Hill assumption (rule of mixtures): no fluctuations in RVE
  - Linear displacement boundary condition (Dirichlet boundary condition): no fluctuation at RVE boundary
    \[ \tilde{\mathbf{u}} = 0 \quad \forall \mathbf{x} \in \partial V \]
  - Periodic boundary condition: periodicity of fluctuation field and anti-periodicity of traction field at RVE boundary
    \[ \tilde{\mathbf{u}}^+ = \tilde{\mathbf{u}}^- \quad \forall \mathbf{x}^+ \in \partial V^+ \text{ and } \forall \mathbf{x}^- \in \partial V^- \]
    \[ \mathbf{t}^+ = -\mathbf{t}^- \quad \mathbf{n}^+ = -\mathbf{n}^- \]
  - Minimal kinematic boundary condition (Neumann boundary condition)
    \[ \mathbf{t} = \mathbf{\bar{\sigma}} \cdot \mathbf{n} \quad \forall \mathbf{x} \in \partial V \]
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**

\[ \bar{\varepsilon} = \frac{1}{V} \int_V \varepsilon \, dV \quad \bar{\varepsilon} = \frac{1}{V} \int_{\partial V} \mathbf{n} \otimes_s \mathbf{u} \, dS \]

- **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:
  - Virtual strain:

\[ \delta \varepsilon = \delta \bar{\varepsilon} + \delta \bar{\varepsilon} \]

  - Equation (***) becomes:

\[ \bar{\sigma} : \delta \bar{\varepsilon} = \frac{1}{V} \int_V \sigma : \delta \varepsilon \, dV \]

  - Stress averaging:

\[ \bar{\sigma} = \frac{1}{V} \int_V \sigma \, dV \]
Coupling of microscopic and macroscopic problem

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

- **Stress averaging and tangent operator**
  - Equilibrium state and Gauss theorem:
    \[
    \bar{\sigma} = \frac{1}{V} \int_V \sigma \, dV \quad \bar{\sigma} = \frac{1}{V} \int_{\partial V} t \otimes x \, dS
    \]
  - Tangent operator:
    \[
    \bar{C} = \partial \bar{\varepsilon} \bar{\sigma}
    \]
Finite element implementation

- 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
    \[ \tilde{u} = N^e(x)q_e \]
    \[ \tilde{\varepsilon} = \nabla \otimes_s \tilde{u} = B^e(x)q_e \]
  - Assemble operator:
    \[ q = \mathcal{A}^m_{e=1} q_e \]
  - Approximation of internal energy:
    \[ \bar{U}^h(\bar{\varepsilon}, q) = \frac{1}{V} \sum_{e=1}^{n_e} \int_{V_e} U(\bar{\varepsilon} + B^e q_e) \, dV \]
Finite element implementation

• RVE boundary condition
  – Linear displacement boundary condition
    • For M nodes on RVE boundary
      \[
      \tilde{u}_i = 0 \quad i = 1..M
      \]

• Partitioning of fluctuation field on RVE boundary
  \[
  q^T = [q_i^T \ q_b^T]
  \]
  \[
  q_i = L_i q
  \]
  \[
  q_b = L_b q
  \]

• Linear constraints on fluctuation displacement
  \[
  q_b = 0
  \]
  \[
  L_b q = 0
  \]
Finite element implementation

- RVE boundary condition
  - Constant traction boundary condition
    - From strain averaging equation
      \[ \frac{1}{V} \int_{\partial V} n \otimes_s \tilde{u} \, dS = 0 \quad (*) \]
    - Assemble on RVE boundary elements
      \[ \frac{1}{V} A_e^{n_e} \int_{(\partial V)_e} n \otimes_s B^e q_e \, dS = 0 \]
  - Linear constraints on fluctuation displacement
    \[ L_b q = 0 \]
Finite element implementation

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

- Periodic mesh: apply on matching node on RVE boundary

\[ \tilde{u}^+ = \tilde{u}^- \quad \forall x^+ \in \partial V^+ \quad \text{and} \quad \forall x^- \in \partial V^- \]

\[ t^+ = -t^- \quad \quad n^+ = -n^- \]

- Linear constraints on fluctuation displacement

\[ q^+ = q^- \]
\[ C_b q_b = 0 \]
\[ C_b L_b q = 0 \]
\[ C q = 0 \]
Finite element implementation

• 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

\[ Cq = 0 \]
Finite element implementation

- **RVE equilibrium state**
  
  - Minimize
    
    $$
    \bar{U}^h(\bar{\varepsilon}, q) = \frac{1}{V} \sum_{e=1}^{n_e} \int_{V_e} U(\bar{\varepsilon} + B^e q_e) dV
    $$
  
  - Subject to:
    
    $$
    C q = g
    $$
  
- **Enforcement by Lagrange multipliers**
  
  - Lagrange function
    
    $$
    \mathcal{L} = \bar{U}^h(\bar{\varepsilon}, q) - \lambda^T (C q - g)
    $$
  
  - Equilibrium state
    
    $$
    \partial_q \bar{U}^h - C^T \lambda = 0
    $$
    
    $$
    C q - g = 0
    $$
  
  - Internal force
    
    $$
    F_{\text{int}} = \partial_q \bar{U}^h
    $$
  
  - Nonlinear system
    
    $$
    F_{\text{int}} - C^T \lambda = 0
    $$
    
    $$
    C q - g = 0
    $$
Finite element implementation

- **Enforcement by Lagrange multipliers**
  - Nonlinear system to solve \( F_{\text{int}} - C^T \lambda = 0 \)
  - \( Cq - g = 0 \)
  - Solve by Newton-Raphson procedure

- **Step 0**
  - \( q^{(0)} = q_0 \)
  - \( \lambda^{(0)} = \lambda_0 \)

- **Step 1**
  - \( \begin{bmatrix} \Delta q^{(i)} \\ \Delta \lambda^{(i)} \end{bmatrix} = -S_T^{-1} \begin{bmatrix} F_{\text{int}}^{(i)} - C^T \lambda^{(i)} \\ Cq^{(i)} - g \end{bmatrix} \)
  - \( S_T - \begin{bmatrix} \partial_q F_{\text{int}}^{(i)} & -C^T \\ C & 0 \end{bmatrix} \)

- **Step 2**
  - \( q^{(i+1)} = q^{(i)} + \Delta q^{(i)} \)
  - \( \lambda^{(i+1)} = \lambda^{(i)} + \Delta \lambda^{(i)} \)

- **Step 3**
  - \( r^{(i+1)} = F_{\text{int}}^{(i+1)} - C^T \lambda^{(i+1)} \)
  - \( \Phi^{(i+1)} = Cq^{(i+1)} - g \)

- **If** \( \max(||r^{(i+1)}||, ||\Phi^{(i+1)}||) < \text{tol} \) **EXIT**

- **else GOTO step 1**
Finite element implementation

- Enforcement by constraint elimination
  - Problem:
    \[ \delta q^T \left( \delta_q \tilde{U}^h \right) = 0 \]
  - Decomposition: dependent part and independent part from constraints
    \[ \delta q^D = S\delta q^I \quad q = \begin{bmatrix} q^I \\ q^D \end{bmatrix} \quad \delta q = L\delta q^I \]
  - New equation of independent part
    \[ (\delta q^I) L^T F_{int}(q^I) = 0 \]
  - Solve by Newton-Raphson procedure
Nested solution scheme

MACRO

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

- Step 2: next load increment at macroscopic problem

- Step 3: next Iteration
  • Solve macroscopic problem
  • Calculate macroscopic forces

- Step 4: convergence
  • If convergence $\rightarrow$ step 2
  • Else $\rightarrow$ step 3

MICRO

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

- RVE analysis
  • Prescribe boundary condition
  • Calculate homogenized stress
  • Calculate homogenized tangent operator
Numerical examples

- **Problem**
  - Vertical displacement
  - Plane strain problem and boundary condition

- **Material**
  - Matrix: \( E_1 = 70 \text{ GPa} \) \( \nu_1 = 0.3 \)
  - Inclusion: \( E_2 = 700 \text{ GPa} \) \( \nu_2 = 0.3 \)
Numerical examples

- **RVE analysis**
  - Macroscopic strain
    \[
    \tilde{\varepsilon} = \begin{bmatrix}
    0 & 0.05 & 0 \\
    0.05 & 0 & 0 \\
    0 & 0 & 0
    \end{bmatrix}
    \]
  - Homogenized stress
    - Linear displacement boundary condition
      \[
      \bar{\sigma} = \begin{bmatrix}
      -0.008 & 3265.030 & 0.000 \\
      3265.030 & -0.280 & 0.000 \\
      0.000 & 0.000 & -0.086
      \end{bmatrix} \text{ (MPa)}
      \]
    - Periodic boundary condition
      \[
      \bar{\sigma} = \begin{bmatrix}
      0.033 & 3177.600 & 0.000 \\
      3177.600 & -0.316 & 0.000 \\
      0.000 & 0.000 & -0.085
      \end{bmatrix} \text{ (MPa)}
      \]
Numerical examples

- RVE analysis
  - Displacement field
  - Von-Mises stress

Linear displacement BC

Periodic BC
Numerical examples

- Multi-scale analysis

Macroscopic finite element mesh

Quadratic triangle
- rule=6
- degree=4

Inclusion Matrix

RVE finite element mesh
Numerical examples

- **Multi-scale analysis**
  - Vertical displacement \( \Delta u = 0.05 \)
  - Reaction force

<table>
<thead>
<tr>
<th></th>
<th>Reaction force</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear displacement BC</td>
<td>3421.955</td>
</tr>
<tr>
<td>Periodic BC</td>
<td>3406.800</td>
</tr>
<tr>
<td>Single scale</td>
<td>3381.519</td>
</tr>
</tbody>
</table>

Plane strain problem and boundary condition
Numerical examples

- 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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