Multiscale Simulations of Composites with Non-Local Damage-Enhanced Mean-Field Homogenization

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Outline

- Introduction
- Mean Field Homogenization
- Nonlocal Approach and Implicit Gradient Formulation
- Ductile Damage in the Matrix of Composite
- Finite Element Implementation
- Validation and Simulation
Introduction

Why Multiscale?

• Materials are multiscale in nature:

Metals

Polymers

Molecular Dynamics

Monte Carlo Method, Statistical Mechanics ...

Continuum Mechanics

$10^{-9}$ m

1 m
/Introduction

Why Multiscale?

• Multiscale Methods for Composites
  ❖ For material design:
    These effective properties are difficult or expensive to measure.
  ❖ For composite structures analysis:
    • Continuum mechanics analysis at Macroscale
      *Accuracy!*
    • Take into account the individual component properties and geometrical arrangements.
      *Expensive, unreachable!*

• Solution:
  ❖ The engineering problems are solved at macroscopic scale with the homogenized properties.
  ❖ The homogenized properties are obtained from the individual component properties and their microstructure.
Problem in finite element simulations

- Finite element solutions for strain softening problems suffer from:
  - The loss the uniqueness and strain localization
  - Mesh dependence
    - Homogenous unique solution
      - Lose of uniqueness
    - Strain localized
      - The numerical results change with the size of mesh and direction of mesh
      - The numerical results change without convergence
Problem in finite element simulations

*Multiscale Methods have this problem too!*

• Solution:
  Introduce high order term in the continuum description
  Strain gradient model, nonlocal model...
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At the macroscale, the problem is a classical continuum mechanics problem (Finite Element method).

At a macroscopic material point the properties of the material correspond to a representative volume element (RVE) of the microstructure.

Basing on

The macro strain $\bar{\varepsilon}$ and stress $\bar{\sigma}$ equal the average strain $\langle \varepsilon \rangle$ and stress $\langle \sigma \rangle$ over a RVE

$$
\langle a \rangle = \frac{1}{V} \int_V a(X) dV
$$
Mean Field Homogenization

- How to get $\mathbf{C}$ in RVE? Such that $\langle \sigma \rangle = \mathbf{C} : \langle \varepsilon \rangle$
  - Direct finite element simulation
  - Semi-analytical mean field homogenization models
    (Voigt, Reuss, Mori-Tanaka, Double-Inclusion, Self-Consistent ...)
- Two-phase composite
  - Volume fraction $\nu_0 + \nu_1 = 1$
    \[
    \begin{align*}
    \langle \sigma \rangle &= \nu_0 \langle \sigma \rangle_{\omega_0} + \nu_1 \langle \sigma \rangle_{\omega_1} \\
    \langle \sigma \rangle_{\omega_1} &= \mathbf{C}_1 : \langle \varepsilon \rangle_{\omega_1} \\
    \langle \sigma \rangle_{\omega_0} &= \mathbf{C}_0 : \langle \varepsilon \rangle_{\omega_0} \\
    \end{align*}
    \]
  - $\langle \varepsilon \rangle = \nu_0 \langle \varepsilon \rangle_{\omega_0} + \nu_1 \langle \varepsilon \rangle_{\omega_1}$
  - $\langle \varepsilon \rangle_{\omega_1} = B^\varepsilon : \langle \varepsilon \rangle_{\omega_0}$

Subscription: 0(matrix) and 1(inclusion)
• Single inclusion problem

\[ \langle \varepsilon \rangle_{\omega_i} = H^\varepsilon (I, \overline{C}_0, \overline{C}_1) : \varepsilon^\infty \]

\( H^\varepsilon \) is single inclusion strain concentration tensor (numerical, analytical)

\[ H^\varepsilon = [I + S : \overline{C}_0^{-1} : (\overline{C}_1 - \overline{C}_0)]^{-1} \]

\( S \) is Eshelby’s tensor

• Multiple inclusion problem

\[ \langle \varepsilon \rangle_{\omega_i} = B^\varepsilon : \langle \varepsilon \rangle_{\omega_0} \quad \langle \varepsilon \rangle_{\omega_i} = A^\varepsilon : \langle \varepsilon \rangle \]

Mori-Tanaka model:

\[ \varepsilon^\infty = \langle \varepsilon \rangle_{\omega_0} \quad \text{and} \quad B^\varepsilon = H^\varepsilon \]
Introduction

Mean Field Homogenization

Nonlocal Approach and Implicit Gradient Formulation

Ductile Damage in the Matrix of Composite

Finite Element Implementation

Validation and Simulation
Nonlocal Approach

• Description

Some variables (\(a\)) are replaced by their weighted (\(\phi\)) average over a characteristic volume (\(V_c\)) to reflect the interaction between neighboring material points.

\[
\tilde{a}(X) = \frac{1}{V_c} \int_{V_c} a(y) \phi(y; X) \, dV
\]

The state variable \(a\) can be strains, internal variables (eg. accumulated plastic strain, damage,...)

**Problem:** Weight function \(w\)? Characteristic volume \(V_c\)?
Implicit Gradient Formulation

- Implicit gradient formulation *:
  - Green’s function $G(y; x) \rightarrow$ weight function $w(y; x)$
    
    $$\tilde{a}(X) = \frac{1}{V_C} \int_{V_C} a(y) \phi(y; X) dV \Rightarrow \tilde{a}(X) - l^2 \nabla^2 \tilde{a} = a(X)$$
  - The natural boundary condition: $$\frac{\partial \tilde{a}}{\partial n} = n_i \frac{\partial \tilde{a}}{\partial X_i} = 0$$

* Peerlings et al., 1996
Composites are anisotropic at the ply scale

- Characteristic size should depend on the direction

\[ \tilde{a}(X) - l^2 \nabla^2 \tilde{a} = a(X) \quad \Rightarrow \quad \tilde{a} - \nabla \cdot (c_g \cdot \nabla \tilde{a}) = a \]

- The natural boundary condition becomes:

\[ (c_g \cdot \nabla \tilde{a}) \cdot n = 0 \]

* Peerlings et al., 1996
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Ductile Damage in the Matrix of Composite

- Damage in matrix only (neglect the Damage in fiber)
- Lemaitre - Chaboche ductile damage model:
  \[ \dot{D} = \left( \frac{Y}{S_0} \right)^n \dot{p} \]
  where \( S_0 \) and \( n \) are the material parameters
  \( Y \) is the strain energy release rate
  \[ Y = \frac{1}{2} \varepsilon^e : E_0 : \varepsilon^e \]
  \( p \) is the accumulated plastic strain
  \[ p = \int \dot{p} \, dt \]
  \[ \dot{p} = \left[ \frac{2}{3} \dot{\varepsilon}^p : \dot{\varepsilon}^p \right]^{1/2} \]

- Nonlocal damage:
  \[ \dot{D} = \begin{cases} 
  0, & \text{if } \tilde{p} \leq p_C \\
  \left( \frac{Y}{S_0} \right)^s \dot{\tilde{p}}, & \text{if } \tilde{p} > p_C 
  \end{cases} \]
  \[ \tilde{p} - \nabla \cdot (c_g \cdot \nabla \tilde{p}) = p \]
Ductile Damage in the Matrix of Composite

• Considering the damage in matrix, the incremental form of stress in composite*:

\[
\delta \sigma = v_0 \delta \sigma_0 + v_I \delta \sigma_I \quad \quad \quad \quad \quad \hat{\sigma}_0 = \sigma_0/(1-D)
\]

\[
\begin{align*}
\delta \sigma &= v_I C_{\text{L}}^{\text{alg}} \cdot \delta \varepsilon_I + v_0 C_0^{\text{algD}} \cdot \delta \varepsilon_0 - v_0 \left( \hat{\sigma}_0 \otimes \frac{\partial D}{\partial \varepsilon_0} \right) \cdot \delta \tilde{\varepsilon} \\
&= \left[ C_{\text{L}}^{\text{algD}} - v_0 \left( \hat{\sigma}_0 \otimes \frac{\partial D}{\partial \varepsilon_0} \right) \cdot \frac{\partial \varepsilon_0}{\partial \tilde{p}} \right] \delta \tilde{p}
\end{align*}
\]

Subscription: 0(matrix) and I(inclusion)

* Doghri I. et al., 2003
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Governing equations

- For implicit gradient enhanced elastic-plasticity

\[ 0 = \nabla \cdot \sigma^T + \rho f \]
\[ \tilde{p} - \nabla \cdot (c_g \cdot \nabla \tilde{p}) = p \]

- Discretization (in each element)

\[
\tilde{p} = N_{\tilde{p}} \tilde{p} \\
U = N_u u
\]

\[
\begin{bmatrix}
K_{uu}^k & K_{u\tilde{p}}^k \\
K_{\tilde{p}u}^k & K_{\tilde{p}\tilde{p}}^k
\end{bmatrix} \begin{bmatrix}
du \\
d\tilde{p}
\end{bmatrix} = \begin{bmatrix}
F_{ext}^k - F_{int}^k \\
F_p^k - F_{\tilde{p}}^k
\end{bmatrix}
\]
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Validation and Simulation

Validation: DNS vs. FE/MFH

- Epoxy-CF (30%)
Notched ply

Epoxy-CF (30%), Transverse loading, single ply

Mesh independent
Validation and Simulation

Comparison with experiments

- Tensile tests with unloading
  Epoxy-CF (60%), in plane loading, [-45/45/45/-45]
Validation and Simulation

Comparison with experiments

- Tensile on open hole specimen
  Epoxy-CF (60%), in plane loading, [-45/45/45/-45]
Validation and Simulation

Comparison with experiments

- Tensile on open hole specimen
  Epoxy-CF (60%), in plane loading, [-45/45/45/-45]
Thank you!

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