Recent Developments in the Micromechanics of Heterogeneous Media: Finite-Volume and Locally-Exact Homogenization Theories

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Rutgers University Graduate Seminar
April 15, 2009

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Definition and Importance

**Micromechanics**: set of techniques for predicting average (effective) response of heterogeneous materials based on the knowledge of constituent properties and geometric arrangement

\[ \bar{\sigma} = C_{\text{eff}} (\bar{\varepsilon} - \bar{\varepsilon}^{\text{th}} - \bar{\varepsilon}^{\text{in}}) \]

- Enabling analysis technology to:
  - identify and select candidate material systems
  - develop engineered materials with desired mechanical and physical properties
  - design/optimize composite structural components (laminated plates, tubes, heat sinks, thermal barriers, etc.)

\[ \bar{\sigma} = \text{average stress} \]
\[ \bar{\varepsilon} = \text{average strain, etc...} \]
\[ C_{\text{eff}} = \text{effective stiffness matrix} \]
Fundamental Micromechanics Problem

- **Localization relations:**
  \[ \bar{\varepsilon}^{(k)} = A^{(k)} \bar{\varepsilon} + D^{(k)} (\bar{\varepsilon}^{(k)\text{pl}}, \bar{\varepsilon}^{(k)\text{th}}) \]

- **Average stress:**
  \[ \bar{\sigma} = \frac{1}{V} \int_V \sigma(x) dV = \frac{1}{V} \sum_{k=1}^N \int_{V_k} \sigma^{(k)}(x) dV_k = \sum_{k=1}^N c_k \bar{\sigma}^{(k)} \]

- **Phase relations:**
  \[ \sigma^{(k)} = C^{(k)} (\varepsilon^{(k)} - \alpha^{(k)} \Delta T) - 2\mu^{(k)} \varepsilon^{(k)\text{pl}} \]

- **Homogenized macroscopic relations:**
  \[ \bar{\sigma} = C^* \bar{\varepsilon} - (\bar{\sigma}^{\text{th}} + \bar{\sigma}^{\text{pl}}) \]

\[ C^* = \sum_{k=1}^N c_k C^{(k)} A^{(k)} \]

\[ \bar{\sigma}^{\text{th}} + \bar{\sigma}^{\text{pl}} = -\sum_{k=1}^N c_k [C^{(k)} D^{(k)} - \Gamma^{(k)} \Delta T - \bar{\sigma}^{(k)\text{pl}}] \]
Examples of Actual Microstructures

- **Unidirectional composites**

  - Graphite/Epoxy
    - Statistically homogeneous
  - SiC/Titanium
    - Periodic (hexagonal)

  Both are transversely isotropic
Microstructural Representations

- **Statistically Homogeneous Microstructures**
  
  RVE $\Rightarrow$ homogenized response characterized by either homogeneous displacement OR homogeneous traction boundary conditions

- **Periodic Microstructures**

  RUC $\Rightarrow$ homogenized response characterized by periodic displacement AND traction boundary conditions
RUC vs RVE: Transverse Shear Response

1 fiber

36 fibers

Displacement bc’s  Traction bc’s  Periodic bc’s
Micromechanics Modeling Approaches

- **Microstructural Detail-Free Schemes**
  - Voigt and Reuss Estimates
  - Self-Consistent and Generalized Self-Consistent Schemes
  - Mori-Tanaka Scheme
  - Three-Phase Mode

- **Statistically Homogeneous Materials**
  - Composite Sphere/Cylinder Assemblage Model

- **Periodic Materials**
  - Approximate models: MOC, GMC
  - Asymptotic Homogenization Theory
    - FEM-based solutions of the unit cell b-v problem
    - HFGMC
    - FV-based solutions of the unit cell problem: FVDAM
    - Elasticity-based, locally-exact solutions of the unit cell b-v problem
Asymptotic Homogenization Theory

- Two scale representation of field quantities

\[
u_i^{(\varepsilon)}(x, y) = u_i^{(0)}(x, y) + \varepsilon u_i^{(1)}(x, y) + O(\varepsilon^2)
\]

where \( y = x/\varepsilon \) \( \rightarrow \)

\[
\frac{\partial}{\partial x_i} \rightarrow \frac{\partial}{\partial x_i} + \frac{1}{\varepsilon} \frac{\partial}{\partial y_i}
\]

- Governing Field Equations:

\[
\frac{\partial}{\partial x_j} \left[ C_{ijkl}(y) \frac{\partial u_k(x, y)}{\partial x_l} \right] + F_i = 0
\]

- Scale Separation

  - \( \varepsilon^{-2} \) order \( \rightarrow \) \( u_i^{(0)}(x, y) = u_i^{(0)}(x) \)

  - \( \varepsilon^{-1} \) order \( \rightarrow \) unit cell b-v problem in terms of \( u_i^{(1)}(x, y) \)

\[
u_i^{(1)}(x, y) = N_i^{mn}(y) \frac{\partial u_m^{(0)}(x)}{\partial x_n}
\]
Asymptotic Homogenization Theory

- $\varepsilon^0$ order $\Rightarrow$ homogenized equation for $u_i^{(0)}(x)$

$$C_{ijkl}^* \frac{\partial^2 u_k^0(x)}{\partial x_j \partial x_l} + F_i^* = 0 \Rightarrow u_i^0(x) = \bar{\varepsilon}_{ij} x_j$$

where

$$C_{ijkl}^* = \frac{1}{V_{\text{ruc}}} \int_{V_{\text{ruc}}} [C_{ijkl}(y) + C_{ijmn}(y) \frac{\partial N_{mn}^k(y)}{\partial y_n}] dV$$

• Observation: consider 0th-order stresses

$$\sigma_{ij}^{(0)}(x, y) = C_{ijkl}(y) \left[ \frac{\partial u_k^0(x)}{\partial x_l} + \frac{\partial u_k^{(1)}(x, y)}{\partial y_l} \right] = C_{ijkl}(y) \left[ \delta_{mk} \delta_{nl} + \frac{\partial N_{mn}^k(y)}{\partial y_l} \right] \frac{\partial u_m^{(0)}(x)}{\partial x_n}$$

$$\Rightarrow \sigma_{ij}^{(0)}(x, y) = C_{ijkl}(y) \left[ \bar{\varepsilon}_{kl} + A'_{klmn}(y) \bar{\varepsilon}_{mn} \right]$$

$$\Rightarrow C_{ijkl}^* = \frac{1}{V_{\text{ruc}}} \int_{V_{\text{ruc}}} [C_{ijkl}(y) + C_{ijmn}(y) A'_{mnkl}] dV$$
Finite-Volume Direct-Averaging Theory

- **Microstructural discretization**

\[ y^{(q)}_i = \sum_{p=1}^{4} N_p(\eta, \xi) y^{(p,q)}_i, \quad i = 2,3 \]

\[ N_1(\eta, \xi) = \frac{1}{4(1-\eta)(1-\xi)}, \ldots \]

- **Displacement field:**

\[ u^{(q)}_i(x, y) = \bar{\varepsilon}_{ij} x_j + u^{(q)}_i(y) \]

\[ u^{(q)}_i = W^{(q)}_{i(00)} + \eta W^{(q)}_{i(10)} + \xi W^{(q)}_{i(01)} + \frac{1}{2} (3\eta^2 - 1) W^{(q)}_{i(20)} + \frac{1}{2} (3\xi^2 - 1) W^{(q)}_{i(02)} \]
Finite-Volume Direct-Averaging Theory

- Surface-averaged displacements

\[ \hat{u}_{i}^{(1,3)} = \frac{1}{2} \int_{-1}^{+1} u'_{i} (\eta, \mp 1) d\eta, \quad \hat{u}_{i}^{(2,4)} = \frac{1}{2} \int_{-1}^{+1} u'_{i} (\pm 1, \xi) d\xi \]

- Surface-averaged tractions

\[ \hat{t}_{i}^{(1,3)} = \frac{1}{2} \int_{-1}^{+1} \sigma_{ji}(\eta, \mp 1) n_{j} d\eta, \quad \hat{t}_{i}^{(2,4)} = \frac{1}{2} \int_{-1}^{+1} \sigma_{ji}(\pm 1, \xi) n_{j} d\xi \]

- Surface-averaged displacement derivative matrices

\[
\begin{bmatrix}
\frac{\partial \hat{u}'_{i}}{\partial y'_{2}} \\
\frac{\partial \hat{u}'_{i}}{\partial y'_{3}}
\end{bmatrix} = \hat{J} \begin{bmatrix}
\frac{\partial \hat{u}'_{i}}{\partial \eta} \\
\frac{\partial \hat{u}'_{i}}{\partial \xi}
\end{bmatrix}, \quad \hat{J}^{-1} = \overline{J} = \frac{1}{2} \int_{-1}^{+1} \int_{-1}^{+1} J d\eta d\xi
\]
Finite-Volume Direct-Averaging Theory

- **Satisfaction of equilibrium equations**
  \[
  \int_{S_q} t dS + \int_{V_q} F dV = 0 \quad \Rightarrow \quad \sum_{p=1}^{4} l_p t^{(q,p)} + \int_{V_q} F dV = 0
  \]

- **Local stiffness matrix construction**
  \[
  \hat{t} = NC\bar{\varepsilon} + K\hat{u}' + AN\Phi^{-1}Z^{pl} - N(\sigma^{th} + \sigma^{pl})
  \]

- **Global stiffness matrix assembly and solution**
  \[
  K\hat{U}' = \Delta C\bar{\varepsilon} + \Gamma + G \quad \Rightarrow \quad \bar{\varepsilon}^{(q)} = A^{(q)}\bar{\varepsilon} + D^{(q)}
  \]

- **Homogenized equations**
  \[
  \bar{\sigma} = C^*\bar{\varepsilon} - (\bar{\varepsilon}^{th} + \bar{\varepsilon}^{pl})
  \]
Effect of Mesh Refinement on Moduli

\[ \frac{E_f}{E_m} = 10 \]

\[ \frac{E_f}{E_m} = 0.01 \]
Effect of Mesh Refinement on Stresses

\( \bar{\sigma}_{12} \neq 0 \)

\( \sigma_{12} \) distributions vs mesh refinement \((24 \times 24, 48 \times 48, 96 \times 96)\)

\( \sigma_{13} \) distributions vs mesh refinement \((24 \times 24, 48 \times 48, 96 \times 96)\)
Mechanics of Wavy Periodic Multilayers

<table>
<thead>
<tr>
<th>Material</th>
<th>Young’s modulus (MPa)</th>
<th>Poisson’s ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soft layers</td>
<td>7,000</td>
<td>0.30</td>
</tr>
<tr>
<td>Hard layers</td>
<td>70,000</td>
<td>0.22</td>
</tr>
</tbody>
</table>
FVDAM Theory vs FE Method

\[ \bar{\sigma}_{22} = 1 \text{ MPa} \]

\[ \sigma_{22} \] distributions

\[ \sigma_{23} \] distributions
Elastic-Plastic Response

σ_{22} distributions at \( \bar{\varepsilon}_{22} = 0.25\% \) (top) and \( \bar{\varepsilon}_{22} = 1.0\% \) (bottom)
Mechanics of Perforated Thin Sheets
Elastic-Plastic Response & Localization

![Graphs showing stress-strain relationship for different hole arrangements](image)

- Circular holes (square array)
- Circular holes (hex array)
- Square holes (square array)
- Hexagonal holes (hex array)
- Slots (hex array)
Locally-Exact Homogenization Theory

- **Displacement field:**
  \[ u_i(x, y) = \bar{E}_{ij} x_j + u'_i(y) \]

- **Interior problem:** locally exact solution → satisfy the Navier’s equations and the fiber-matrix continuity in cylindrical coordinates

- **Exterior problem:** solved in Cartesian coordinates using a variational principle
Interior Problem

- **Locally exact solutions**

\[
u'_z = H^{(f,m)}_{01} + \sum_{n=1}^{N} \left( \zeta^n H^{(f,m)}_{n1} + \zeta^{-n} H^{(m)}_{n3} \right) \cos(n\theta) + \left( \zeta^n H^{(f,m)}_{n2} + \zeta^{-n} H^{(m)}_{n4} \right) \sin(n\theta)
\]

\[
u'_r = \zeta F^{(f,m)}_{01} + \zeta^{-1} F^{(m)}_{02} + F^{(f,m)}_{12} \cos \theta + G_{12}^{(f,m)} \sin \theta \\
+ \sum_{n=2}^{N} \sum_{j=1}^{4} \zeta^p_{nj} \left[ F^{(f,m)}_{nj} \cos(n\theta) + G^{(f,m)}_{nj} \sin(n\theta) \right]
\]

\[
u'_\theta = -F^{(f,m)}_{12} \sin \theta + G_{12}^{(f,m)} \cos \theta + \sum_{n=2}^{N} \sum_{j=1}^{4} \beta_{nj} \zeta^p_{nj} \left[ F^{(f,m)}_{nj} \sin(n\theta) - G^{(f,m)}_{nj} \cos(n\theta) \right]
\]

- **Fiber/matrix continuity**

\[
A^m_n F^m_n = A^f_n F^f_n + \delta_{n2} A_o \left( \bar{\varepsilon}_{22} - \bar{\varepsilon}_{23} \right)
\]

\[
A^m_n G^m_n = A^f_n G^f_n + \delta_{n2} A_o \left( 2\bar{\varepsilon}_{23} \right)
\]

\[
H^m_n = A^f_1 H^f_n + \delta_{n1} A_2 \left[ 2\bar{\varepsilon}_{12} 2\bar{\varepsilon}_{12} \right]^T
\]
Exterior Problem

- Balanced Variational principle

\[ H = \frac{1}{2} \int_V \sigma_{ij} \varepsilon_{ij} \, dV - \int_{S_u} T_i u_i^o \, dS - \int_{S_r} T_i^o u_i \, dS \]

- Periodic boundary conditions

\[ u_i(x+d) = u_i(x) + \varepsilon_{ij} d_j \quad \Rightarrow \quad u_i'(x+d) = u_i'(x) \]
\[ T_i(x+d) + T_i(x) = 0 \]

- Minimization

\[ \int_{S_u} \delta T_i (u_i - u_i^o) \, dS + \int_{S_r} \delta u_i (T_i - T_i^o) \, dS = 0 \]

- Global system of equations:

\[ A x = B \bar{\varepsilon} \]
Convergence Characteristics

\[ \frac{E_f}{E_m} = 10 \]
Comparison of Homogenized Moduli

\[ \frac{E_f}{E_m} = 10 \]
Comparison of Local Stress Fields

Loading by $\bar{\varepsilon}_{23} \neq 0$

$\sigma_{23}$

$\sigma_{22}$
Comparison of Boundary Deformations

Transverse Normal Loading

Transverse Shear Loading

Stiff Fiber

Porosity

Legend:
- Dashed blue line: Undeformed
- Red line: Deformed - Analytical
- Black circle: Deformed - FEA
Multi-Inclusion Unit Cells – 1st Steps

- Multi-scale analysis
  - Large fiber, $v_f = 40\%$
  - Small fiber, $v_f = 1\%$

FEA Mesh – 9,752 elements $\rightarrow$ 39,811 DOFs
Series - 12 harmonics per subvolume $\rightarrow$ 188 Coefficients
Comparison of Stress Fields

Loading by $\bar{\varepsilon}_{22} \neq 0$

(a) Balanced Variational Principle
(b) FEA
Comparison of Stress Fields

Loading by $\bar{\varepsilon}_{23} \neq 0$
Summary & Things to Do

- FVDAM produces stable macroscopic response even with relatively coarse mesh discretization
- High-fidelity stress fields with FEM accuracy require greater discretization
- FVDAM is the more developed of the two methods, with "apparently" greater potential
- LEXHT in early stages of development with promising results
- Extension to multi-inclusion unit cells with arbitrary distributions a major step
- Possibility of three-dimensional analysis of unit cells with ellipsoidal inclusions