Limit State of Heterogeneous Materials under Thermo-mechanical Loading

M. Chen, A. Hachemi, D. Weichert
A mechanical structure or structural element made of composite materials operates beyond the elastic limit:

1) Determination of material properties
2) Variable loads with unknown evolution in time
3) Temperature dependent material properties
4) Space loads

Direct methods combined with homogenization technique
1) Prediction of the global material properties by using homogenization theory
2) Direct methods give information on serviceability without calculating the evolution of mechanical field quantities.
3) & 4): ??
Direct methods applied to composites
  • Elements of homogenization theory
  • FEM & Optimization

Temperature dependent material properties
  • Temperature dependent yield strength
  • Temperature dependent Young‘s Modulus

3D RVE under space loads
  • Homogenized material properties

Numerical examples
  • Comparison of boundary condition
  • Temperature-dependent material properties under thermal loading
  • Ellipsoidal inclusion composites under space loads

Conclusions
DIRECT METHODS APPLIED TO COMPOSITES

General methodology: multiscale method

Micro-/Mesoscopic Level
---------------------------------------
Numerical Model for limit and shakedown analysis of RVE
Numerical Solution for limit and shakedown problem (FEM & Optimization)

Macroscopic Level
----------------------------------------
Prediction of elastic and plastic material properties
Comparison of loading carrying capacity of composites with different fiber distributions, types, ratio.

➢ Assumptions
• perfect interface
• at least one ductile phase
Homogenization theory

- Concept of representative volume element (RVE)

\[ \xi = x/\theta, \quad \theta: \text{a small parameter} \]

- Average field quantities *

\[ \Sigma(x) = \frac{1}{V} \int_V \sigma(\xi) \, dV = \langle \sigma(\xi) \rangle \]

\[ E(x) = \frac{1}{V} \int_V \varepsilon(\xi) \, dV = \langle \varepsilon(\xi) \rangle \]

DIRECT METHODS APPLIED TO COMPOSITES

Static direct methods for periodic composites *

\[ \Sigma = \frac{1}{V} \int \left( \alpha \sigma_E + \bar{\rho} \right) dV = \frac{1}{V} \int \alpha \sigma_E dV + \frac{1}{V} \int \bar{\rho} dV \quad \text{with} \quad \frac{1}{V} \int \bar{\rho} dV = 0 \]

Definitions of macroscopic stresses **

- Homogenized elastic stress : \( \Sigma_{EL} = \alpha_{EL} \langle \sigma^E \rangle \)
- Homogenized shakedown stress : \( \Sigma_{SD} = \alpha_{SD} \langle \sigma^E \rangle \)
- Homogenized limit stress : \( \Sigma_{LM} = \alpha_{LM} \langle \sigma^E \rangle \)

Homogenized material parameters

- Elastic mechanical parameters
- Thermal parameters
- Plastic mechanical parameters

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**DIRECT METHODS APPLIED TO COMPOSITES**

**Localization problem – Boundary conditions** *

- **Strain method**
  Uniform strain is imposed on $\partial V$: $u = E \cdot \xi$ on $\partial V$

- **Stress method**
  Uniform stress is imposed on $\partial V$: $\sigma \cdot n = \Sigma \cdot n$ on $\partial V$

- **Periodicity**
  Anti-periodicity of stress: $\sigma \cdot n$ anti-periodic on $\partial V$
  Decomposition of local strain: $\varepsilon(u) = E + \varepsilon(u^{\text{per}}) = E + \varepsilon^{\text{per}}$
  Average of $\varepsilon^*$ over the RVE: $\langle \varepsilon^{\text{per}} \rangle = 0$

**Periodic composites** **

- Periodic composite problem $\mathcal{P}$:
  \[
  \begin{cases}
  \text{div } \sigma^E = 0 & \text{in } V \\
  \sigma^E = \mathbf{d} : (E + \varepsilon^{\text{per}}) & \text{in } V \\
  \sigma^E \cdot n & \text{anti-periodic on } \partial V \\
  \varepsilon^{\text{per}} & \text{periodic on } \partial V \\
  \langle \varepsilon \rangle = E & \text{or } \langle \sigma \rangle = \Sigma
  \end{cases}
  \]

- Prescribed problem $\mathcal{P}^{\text{pres}}$:
  \[
  \begin{cases}
  \text{div } \bar{\rho} = 0 & \text{in } V \\
  \bar{\rho} \cdot n & \text{anti-periodic on } \partial V \\
  \langle \varepsilon^{\text{per}} \rangle = 0
  \end{cases}
  \]

---


Implementation of boundary conditions

- **Strain method**
  - All faces remain planar to maintain periodicity.
  - Macroscopic displacement: $\Delta L_i$

- **Periodic constraint**
  - Constraint: $u'_i - u_i + u^d_i = 0$
  - $u'_i, u_i$: displacements of relative opposite periodic node pairs
  - $u^d_i$: displacement of dummy node
  - Macroscopic displacement: $u^d_i$

\[\text{DIRECT METHODS APPLIED TO COMPOSITES}\]

- All faces remain planar to maintain periodicity.
- Macroscopic displacement: $\Delta L_i$

- Constraint: $u'_i - u_i + u^d_i = 0$
- $u'_i, u_i$: displacements of relative opposite periodic node pairs
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- Macroscopic displacement: $u^d_i$

DIRECT METHODS APPLIED TO COMPOSITES

Finite element discretization

Principle of virtual work

\[ \int_V \{\delta \varepsilon\}^T \{\alpha \sigma^E + \bar{\rho}\} \, dV = V \Sigma: \delta E \]

➢ Mathematic formulation of shakedown problem

- Objective function \( \max \alpha \)
- Variables \([C]\{\bar{\rho}\} = 0 \]
- Linear equality constraints \(F[\alpha \sigma_i^E (P_k) + \bar{\rho}_i, \sigma_{yi}] \leq 0 \)
- Nonlinear inequality constraints \(i \in [1, NGS], k \in [1, 2^n] \)

- Load factor \( \alpha \)
- \( \alpha \) and residual stress field \( \bar{\rho} \)
- Self-equilibrated condition
- Yield condition

Large-scale optimization

- Algorithm
  - Augmented Lagrangian method
  - Sequential quadratic programming
  - Interior Point Method
- Software Packages
  - LANCELOT, ...
  - SNOPT, NPSOL, NLPQL
  - IPOPT*, IPDCA**, IPSA***...
  - CPLEX, MOSEK......

EXTENSION 1: Temperature Dependent Material Properties

**Constant $E$, Constant $\sigma_Y$**

Classical shakedown formulation:

\[
\max \alpha \\
\begin{cases}
  \{C\}\{\bar{\rho}\} = 0 \\
  F[\alpha\sigma^E(P_k) + \bar{\rho}, \sigma_Y] \leq 0
\end{cases}
\]

**Constant $E$, Temperature dependent $\sigma_Y(T)$**

Shakedown occurs, only if, there exists a time-independent residual stress field $\bar{\rho}$ with the superposition of elastic stresses $\sigma^E$, does not violate the *temperature dependent yield condition*:

\[
F[\alpha\sigma^E(P_k) + \bar{\rho}, \sigma_Y[T]] \leq 0 \quad \text{with: } T = T_a + \alpha\Delta T
\]

$T_a$ : ambient temperature; $\Delta T$ : initial thermal loading; $\sigma_Y[T]$ : continuous function of temperature.

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EXTENSION 1: Temperature Dependent Material Properties

**Latest analogous study: two-bar system with** $E(T)$ *

**Temperature dependent $E(T)$, Constant $\sigma_Y$**

Shakedown occurs, when at temperature $T$, there exist a time-independent residual stress field $\bar{\rho}(T)$ with the superposition of thermo-elastic stress response $\sigma^E(T)$ does not violate the yield condition:

$$F[\sigma^E(T, P_k) + \bar{\rho}(T), \sigma_Y] \leq 0$$

with: $T = T_a + \alpha \Delta T$

**Temperature dependent $E(T)$, Temperature independent $\sigma_Y(T)$**

Shakedown occurs, when at temperature $T$, there exist a time-independent residual stress field $\bar{\rho}(T)$ with the superposition of thermo-elastic stress response $\sigma^E(T)$ does not violate the temperature dependent yield condition:

$$F[\sigma^E(T, P_k) + \bar{\rho}(T), \sigma_Y[T]] \leq 0$$

with: $T = T_a + \alpha \Delta T$


Self-equilibrium!!
**EXTENSION 1: Temperature Dependent Material Properties**

Illustration of shakedown analysis with $E(T)$

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Young's Modulus</th>
<th>Thermal Loading</th>
<th>Elastic stress field</th>
<th>Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_0$</td>
<td>$E(T_0)$</td>
<td>$\Delta T_0$</td>
<td>$\sigma^E(T_0)$</td>
<td>$\alpha_0$</td>
</tr>
<tr>
<td>$T_1 = T_0 + \alpha_0 \Delta T_0$</td>
<td>$E(T_1)$</td>
<td>$\Delta T_1 = \alpha_0 \Delta T_0$</td>
<td>$\sigma^E(T_1)$</td>
<td>$\alpha_1$</td>
</tr>
<tr>
<td>$T_2 = T_0 + \alpha_1 \Delta T_1$</td>
<td>$E(T_2)$</td>
<td>$\Delta T_2 = \alpha_1 \Delta T_1$</td>
<td>$\sigma^E(T_2)$</td>
<td>$\alpha_2$</td>
</tr>
<tr>
<td>$\vdots$</td>
<td>$\vdots$</td>
<td>$\vdots$</td>
<td>$\vdots$</td>
<td>$\vdots$</td>
</tr>
<tr>
<td>$T_i = T_0 + \alpha_{i-1} \Delta T_{i-1}$</td>
<td>$E(T_i)$</td>
<td>$\Delta T_i = \alpha_{i-1} \Delta T_{i-1}$</td>
<td>$\sigma^E(T_i)$</td>
<td>$\alpha_i$</td>
</tr>
</tbody>
</table>

If: $|\alpha_i - 1| < \text{Tol}$, Stop!

**Self-equilibrated condition!!**

Shakedown load factor: $\alpha_{SD} = \prod_{0}^{i} \alpha_i$
Numerical implementation of SD with temperature dependent $E(T)$ and $\sigma_Y(T)$

**PLATFORM: MATLAB**

1. **Call ANSYS**
2. **Construction of $[C]$**
   - Elastic Stress $\sigma^E(T)$
   - Yield strength $\sigma_Y(T)$
3. **Call AMPL**
   - Solver: IPOPT/CPLEX
   - $T_{i+1} = \alpha_i T_i$
   - $E(T_{i+1})$

**Flowchart:**
- $\alpha_i$
- $|\alpha_i - 1| < \text{tol}$
- **Y**: Continue
- **N**: Stop

**Packages:**
1. **Package 1: ANSYS**
   - *Initial data files*
2. **Package 2: MATLAB**
   - *Construction $[C]$*
3. **Package 3: AMPL+Solver**
   - *Optimization*
**EXTENSION 2: Space Load**

**Definition of load space**

A finite number $n$ of types of independent loads:

$$ P(x, t) = P[\beta_s(t), x] \quad x \in V \text{ or } S_p; \ s = 1, \ldots, r; \ \beta^-_s \leq \beta_s(t) \leq \beta^+_s \quad s = 1, \ldots, n $$

Loading domain $P$ can be described by a $n$-dimensional load space.

$$ P(x, t) = \left\{ P \mid P = \sum_{s=1}^{n} \mu_s(t) P_{0i}(x), \quad \mu_s(t) \in [\mu^-_i, \mu^+_i] \right\} $$

---

Numerical discretization of space load domain

3 independent loads: $2^n = 3$

8 Load vertices:

(P1) -> SE1=0
(P2) -> SE2 = sinθ · cosφ · $\sigma_E^1$ (L1)
(P3) -> SE3 = sinθ · sinφ · $\sigma_E^2$ (L2)
(P4) -> SE4 = SE2 + SE3
(P5) -> SE5 = SE1 + cosθ · $\sigma_E^3$ (L3)
(P6) -> SE6 = SE2 + cosθ · $\sigma_E^3$ (L3)
(P7) -> SE7 = SE3 + cosθ · $\sigma_E^3$ (L3)
(P8) -> SE8 = SE4 + cosθ · $\sigma_E^3$ (L3)

EXTENSION 2: Space Load

$$\max \alpha \quad \begin{bmatrix} [C] \{ \bar{p} \} = 0 \\
F[\alpha \sigma_k^E(P_k) + \bar{p}_i, \sigma_{Yi}] \leq 0 \\
i \in [1, NGS], k \in [1, 8]$$

Latest analogous study: Homogeneous structure under space loads *

Reformulation of the optimization problem: Efficiency!

Refer.: Presentation from G. Chen “A statistical evaluation of the yield, ultimate strength and fatigue limit of WC-Co using a direct approach”

The original problem can be formulated into an equivalent but more efficient form by adopting \{\mathbf{u}, \mathbf{x}\} as variable:

\[
\left( P_{\text{3D,Perfect}}^{\text{3D}} \right) \quad \max_{\mathbf{p}} \alpha
\]

\[
[C][\mathbf{p}] = 0, \text{ where } [C] \in \mathbb{R}^{3NK \times 6NGS}
\]

\[
f(\alpha \sigma_i^E(\bar{P}_k) + \bar{P}_i, \sigma_i^Y) \leq 0
\]

\[i \in [1, NGS], k = 1 \text{ or } 2\]

\[
\left( P_{\text{Reform,Perfect}}^{\text{3D}} \right) \quad \max_{\alpha}
\]

\[\sum_{n=1}^{NGS} A_n \mathbf{u}_n^1 + Bx^1 - \alpha \mathbf{w}^1 = 0,
\]

\[[A_n] \in \mathbb{R}^{3NK \times 5}, [B] \in \mathbb{R}^{3NK \times NGS}, \mathbf{w}^{3NG} = [C][\sigma(\bar{P}_1)]
\]

\[
\mathbf{u}_n^2 - \mathbf{u}_n^1 = [U]\{\sigma_i^{2,E} - \sigma_i^{1,E}\}
\]

\[\|\mathbf{u}_n^{1,2}\| \leq 1\]

Solver: CPLEX
NUMERICAL EXAMPLE 1

Comparison of boundary conditions

• Schematic illustration

Periodicity in plane 1-2

• Geometry and finite element model

<table>
<thead>
<tr>
<th></th>
<th>Dimension mm</th>
<th>Fiber ratio</th>
<th>Nr. Elements</th>
<th>Nr. Nodes</th>
<th>Nr. Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>RVE 1</td>
<td>100×100</td>
<td>40</td>
<td>540</td>
<td>1122</td>
<td>25921</td>
</tr>
<tr>
<td>RVE 2</td>
<td>100×100</td>
<td>40</td>
<td>828</td>
<td>1752</td>
<td>39745</td>
</tr>
</tbody>
</table>

• Material properties: Temperature independent

<table>
<thead>
<tr>
<th></th>
<th>α</th>
<th>E</th>
<th>ν</th>
<th>σ_Y</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix (Al)</td>
<td>25.5 × 10^{-6}</td>
<td>70e3</td>
<td>0.3</td>
<td>80</td>
</tr>
<tr>
<td>Fiber (A_13O_2)</td>
<td>7.0 × 10^{-6}</td>
<td>370e3</td>
<td>0.3</td>
<td>2000</td>
</tr>
</tbody>
</table>
### NUMERICAL EXAMPLE 1

- Thermal loading: $\Delta T = 20^\circ C$

<table>
<thead>
<tr>
<th>Approach</th>
<th>Deformation</th>
<th>Macroscopic Disp. &amp; Load factors</th>
<th>Deformation</th>
<th>Macroscopic Disp. &amp; Load factors</th>
</tr>
</thead>
</table>
| ![Approach Diagram](image1) | ![Deformation Diagram](image2) | $\Delta U_1 = 1.1012$  
$\Delta U_2 = 1.1012$  
$\alpha_{EL} = 1.5105$  
$\alpha_{SD} = 3.0126$ | ![Deformation Diagram](image3) | $\Delta U_1 = 1.0893$  
$\Delta U_2 = 1.0942$  
$\alpha_{EL} = 1.1520$  
$\alpha_{SD} = 2.3045$ |
| ![Approach Diagram](image4) | ![Deformation Diagram](image5) | $\Delta U_1 = 1.1012$  
$\Delta U_2 = 1.1012$  
$\alpha_{EL} = 1.5105$  
$\alpha_{SD} = 3.0126$ | ![Deformation Diagram](image6) | $\Delta U_1 = 1.0948$  
$\Delta U_2 = 1.0899$  
$\alpha_{EL} = 1.1695$  
$\alpha_{SD} = 2.3385$ |
NUMERICAL EXAMPLE 2

Temperature dependent material properties

- Material properties

<table>
<thead>
<tr>
<th></th>
<th>α 1/°C</th>
<th>E  MPa</th>
<th>ν</th>
<th>σ_Y MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix (Al)</td>
<td>25.5x10^{-6}</td>
<td>E^m(T)</td>
<td>0.3</td>
<td>σ_Y^m(T)</td>
</tr>
<tr>
<td>Fiber (A_13O_2)</td>
<td>7.0x10^{-6}</td>
<td>370e3</td>
<td>0.3</td>
<td>2000</td>
</tr>
</tbody>
</table>

- Assumption

  1. Fiber: temperature independent
  2. Matrix: temperature dependent

- Matrix

  \[ \sigma_Y^m(T) = 100 - 0.5T \]
  \[ = 100 - 0.5(\alpha \Delta T + T_a) \]
  \[ E^m(T) = -80T + 70000 \]

- Thermal loading

  \[ T_a = 0°C \quad \Delta T = 20°C \]

- Notations

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NE=144</td>
<td>Nr. of elements</td>
</tr>
<tr>
<td>NEM=48</td>
<td>Nr. of elements for matrix</td>
</tr>
<tr>
<td>NEF=96</td>
<td>Nr. of elements for fiber</td>
</tr>
<tr>
<td>NK=332</td>
<td>Nr. of nodes</td>
</tr>
<tr>
<td>NGE=8</td>
<td>Nr. of Gauss Point of each solid element</td>
</tr>
<tr>
<td>NGS=NE*NGE</td>
<td>Nr. of total Gauss Points</td>
</tr>
<tr>
<td>NGM=NEF*NGE</td>
<td>Nr. of Gauss Points for matrix</td>
</tr>
<tr>
<td>NGSF=NEF*NGE</td>
<td>Nr. of Gauss Points for fiber</td>
</tr>
</tbody>
</table>
# NUMERICAL EXAMPLE 2

- **Numerical results**

<table>
<thead>
<tr>
<th>Model</th>
<th>Shakedown Formulation</th>
<th>Remark</th>
<th>$\alpha_{SD}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Model 1</strong></td>
<td>$E^m$</td>
<td>$\sigma^m_Y$</td>
<td>$\max \alpha$</td>
</tr>
<tr>
<td>$E^m$</td>
<td>$\sigma^m_Y$</td>
<td>$F(\alpha \sigma^E_i (P_k) + \overline{\rho}<em>i, \sigma^m</em>{Y_i}) \leq 0$</td>
<td>$i \in [1, NGS]$</td>
</tr>
<tr>
<td><strong>Model 2</strong></td>
<td>$E^m$</td>
<td>$\sigma^m_Y(T)$</td>
<td>$\max \alpha$</td>
</tr>
<tr>
<td>$E^m$</td>
<td>$\sigma^m_Y(T)$</td>
<td>$F(\alpha \sigma^E_i (P_k) + \overline{\rho}<em>i, \sigma^m</em>{Y_i}(T)) \leq 0$</td>
<td>$i \in [1, NGS]$</td>
</tr>
<tr>
<td><strong>Model 3</strong></td>
<td>$E^m(T)$</td>
<td>$\sigma^m_Y$</td>
<td>$\max \alpha$</td>
</tr>
<tr>
<td>$E^m(T)$</td>
<td>$\sigma^m_Y$</td>
<td>$F(\alpha \sigma^E_i (T, P_k) + \overline{\rho}<em>i(T), \sigma^m</em>{Y_i}(T)) \leq 0$</td>
<td>$i \in [1, NGS]$</td>
</tr>
<tr>
<td><strong>Model 4</strong></td>
<td>$E^m(T)$</td>
<td>$\sigma^m_Y(T)$</td>
<td>$\max \alpha$</td>
</tr>
<tr>
<td>$E^m(T)$</td>
<td>$\sigma^m_Y(T)$</td>
<td>$F(\alpha \sigma^E_i (T, P_k) + \overline{\rho}<em>i(T), \sigma^m</em>{Y_i}(T)) \leq 0$</td>
<td>$i \in [1, NGS]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$E^m(T) = -80T + 70e3$</td>
</tr>
</tbody>
</table>
### NUMERICIAL EXAMPLE 2

• Discussion: Efficiency & Convergency

Laptop Configuration:

Processor: Intel(R) Core(TM) i7-2620M CPU @ 2.70GHz
Installed memory (RAM): 8.00 GB (7.89 GB usable)
System type: 64-bit Operating System

<table>
<thead>
<tr>
<th>Model 3 --- $E^m(T)$, $\sigma_Y^m$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model 4 --- $E^m(T)$, $\sigma_Y^m(T)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
</tbody>
</table>

NUMERICL EXAMPLE 3

Ellipsoidal inclusion composites under space loads

- Material properties

<table>
<thead>
<tr>
<th></th>
<th>$\alpha$</th>
<th>$E$</th>
<th>$\nu$</th>
<th>$\sigma_Y$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1/°C</td>
<td>MPa</td>
<td></td>
<td>MPa</td>
</tr>
<tr>
<td>Matrix (Al)</td>
<td>$25.5 \times 10^{-6}$</td>
<td>70e3</td>
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<td>$7.0 \times 10^{-6}$</td>
<td>370e3</td>
<td>0.3</td>
<td>2000</td>
</tr>
</tbody>
</table>

- FEM model

- Loading condition

3 independent loads:
L1: Ux=U0; Uy=Uz=0;
L2: Uy=U0; Ux=Uz=0;
L3: Uz=U0; Ux=Uy=0. with U0=0.02 mm

RVE: 100mm*100mm*100mm
Ellipsoid: a=1.5b
Fiber ratio : 10%
NUMERICAL EXAMPLE 3

- Shakedown domain of ellipsoidal inclusion composites
NUMERICAL EXAMPLE 3

- Homogenized material properties of ellipsoidal inclusion composites

- Periodicity in space 1-2-3
- Constitutive law of orthotropic elastic material
CONCLUSIONS

Summary

• Application of direct methods to composites. Comparison between boundary conditions. Extension to temperature dependent material model and three independent loads.

• Uniform platform (MATLAB) is developed. The interaction of FEM (ANSYS) and optimization software (AMPL+Solver) improved the simplicity and efficiency of numerical calculation.

• Prediction of mechanical material properties of particle inclusion composites based on homogenization theory.

Perspectives

• Mathematical proof for convergence for shakedown condition with temperature dependent Young’s modulus model should be improved.

• Application on non-periodic composites with temperature independent material properties which requires large improvement of the optimization efficiency.
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Dr. J.-W. Simon, K. Nikolaou

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