HOMOGENIZATION METHOD APPLIED TO THE DEVELOPMENT OF COMPOSITE MATERIALS

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• Introduction to Homogenization Method
• Homogenization of FGM Materials
• Topology Optimization Method
• Material Design Concept
• Conclusions and Future Trends
Concept of Homogenization Method

Homogenization method allows the calculation of composite effective properties knowing the topology of the composite unit cell.

Example of application:

- **a)** perforated beam
  - **F** → **unit cell** → **Homogenized Material**

- **b)** brick wall
  - **F** → **unit cell** → **Homogenized Material**
Concept of Homogenization Method

It allows the replacement of the composite medium by an “equivalent” homogeneous medium to solve the global problem.

Advantage in relation to other methods:

- it needs only the information about the unit cell
- the unit cell can have any complex shape

Complex unit cell topologies → implementation using FEM

Analytical methods

- Mixture rule models - no interaction between phases
- Self-consistent methods - some interaction, limited to simple geometries
- **Periodic composites**;
- Asymptotic analysis, mathematically correct;
- Scale of microstructure must be very small compared to the size of the part;
- Acoustic wavelength larger than unit cell dimensions. (Dispersive behavior can also be modeled)
Literature Review

Theory development (elastic medium):
• Sanchez-Palencia (1980) - France
• De Giorgi and Spagnolo (1973) (G-convergence) - Italy
• Duvaut (1976) and Lions (1981) - France
• Bakhvalov and Panasenko (1989) - Soviet Union

Numerical Implementation using FEM:
• Léné (1984) - France
• Guedes and Kikuchi (1990) - USA

Dispersive behavior:
• Turbé (1982) - France
Extension to Other Fields

- flow in porous media - Sanchez-Palencia (1980)
- conductivity (heat transfer) - Sanchez-Palencia (1980)
- viscoelasticity - Turbé (1982)
- biological materials (bones) - Hollister and Kikuchi (1994)
- electromagnetism - Turbé and Maugin (1991)
- piezoelectricity - Telega (1990), Galka et al. (1992), Turbé and Maugin (1991), Otero et al. (1997)

etc …
• Properties $c_{ijkl}$ are Y-periodic functions (Y - unit cell domain).

• Asymptotic expansion:
  - displacements: $u^\varepsilon = u_0(x) + \varepsilon u_1(x, y)$
  where $y = x/\varepsilon$ and $\varepsilon > 0$ is the composite microstructure microscale, and $u_1$ is Y-periodic first order variation term.
Theoretical Formulation

\[ u^\varepsilon = u_0(x) + \varepsilon u_1(x, y); \quad y = x/\varepsilon \]

Energy Functional for the Medium

Theory of Asymptotic Analysis

microscopic equations (\(\delta u_1(x, y)\) terms)

macroscopic equations (\(\delta u_0(x)\) terms)

FEM solution of microscopic equations for \(\chi\)

Due to linearity: \(u_1 = \chi(x, y)\varepsilon(u_0(x))\)

where \(\chi\) is Y-periodic characteristic functions of the unit cell
Substitute in the system of microscopic equations ($\chi$):

$$\chi_i \equiv \sum_{l=1}^{\text{NN}} N_l \chi_{il} \quad I=1,\text{NN} \quad \text{NN} = \begin{cases} 4 \text{ nodes} & \rightarrow \text{ 2D case} \\ 8 \text{ nodes} & \rightarrow \text{ 3D case} \end{cases}$$

Bilinear (2D) and trilinear (3D) interpolation functions

Substitute in the system of microscopic equations ($\chi$):

FEM system of equations:

$$\begin{bmatrix} K \end{bmatrix} \{ \chi^{(mn)} \} = \{ F^{(mn)} \}$$

load cases

\begin{align*}
\text{3 for 2D} \\
\text{6 for 3D}
\end{align*}
Homogenization Implementation

FEM model and Data Input

Assembly of Stiffness Matrix

Solver

Number of load cases:

\[ \begin{cases} 
6 \text{ for 3D} \\
3 \text{ for 2D} 
\end{cases} \]

periodicity conditions enforced in the unit cell

Calculation of Homogenized Coefficients

\( c_H \)
Physical Concept of Homogenization

Load Cases (2D model)

Solutions using FEM

Calculation of effective properties ($c_H$)
Example

Homogenization of composite material with solid and fluid phases

Discretized Unit Cell

Solid phase

Fluid phase
Example

Homogenization of woven fabric composites

Discretized Unit Cell

230,000 brick elements

230,000 brick elements
Example

Homogenization of bone microstructure

(Hollister and Kikuchi - 1997)
Example

“Representative Volume Element (RVE)” concept

Micrograph of Metal Matrix Composites (MMC)

RVE unit cell

Cr (fiber) - NiAl (matrix)

There must be “statistic” periodicity !!!
Homogenization for Coupled Field Materials

Example: Piezoelectric Material

- Force
- Displacement
- Mechanical Energy
- Piezoelectric Material
- Electric potential
- Electric charge
- Electrical Energy

Examples: Quartz (natural)
- Ceramic (PZT5A, PMN, etc…)
- Polymer (PVDF)

Applications: Pressure sensors, accelerometers, actuators, acoustic wave generation (ultrasonic transducers, sonars, and hydrophones), etc...
Constitutive Equations of Piezoelectric Medium

\[
\begin{align*}
T_{ij} &= c_{ijkl}^E S_{kl} - e_{kij} E_k \\
D_i &= \varepsilon_{ik}^S E_k + e_{ikl} S_{kl}
\end{align*}
\]

- \(T_{ij}\) - stress
- \(S_{kl}\) - strain
- \(E_k\) - electric field
- \(D_i\) - electric displacement
- \(c_{ijkl}^E\) - stiffness property
- \(e_{kij}\) - piezoelectric strain property
- \(\varepsilon_{ik}^S\) - dielectric property
• Properties $c_{ijkl}^E$, $e_{ijk}$, and $\varepsilon_{ij}^S$ are $Y$-periodic functions ($Y$ - unit cell domain).

• Asymptotic expansion:
  - displacements: $u^\varepsilon = u_0(x) + \varepsilon u_1(x, y)$
  - electric potential: $\phi^\varepsilon = \phi_0(x) + \varepsilon \phi_1(x, y)$

where $y = x/\varepsilon$ and $\varepsilon > 0$ is the composite microstructure microscale, and $u_1$ and $\phi_1$ are $Y$-periodic first order variation terms.

Telega (1990), Galka et al. (1992), and Turbé and Maugin (1991)
Homogenization Implementation

Load Cases (2D model)

Unit Cell

Calculation of effective properties ($c^E_H$, $e_H$, and $\varepsilon^S_H$)

Solutions using FEM

periodicity conditions enforced in the unit cell

Number of load cases

9 for 3D model
5 for 2D model
Example

3D Piezocomposite Unit Cell

polymer  piezoceramic

“circular inclusion”

“square inclusion”

“staggered formation”

Performance quantity

\[ \text{Ceramic Volume Fraction (\%)} \]

\[ d_h (\text{pC/N}) \]

\[ \begin{align*}
\text{Rectangular inclusion} & : \ldots \\
\text{Circular inclusion} & : \ldots \\
\text{Rectangular inclusion (hex.)} & : \ldots
\end{align*} \]
FGM materials possess continuously graded properties with gradual change in microstructure which avoids interface problems, such as, stress concentrations.
Collaboration USP/UIUC

University of São Paulo

University of Illinois at Urbana-Champaign

• Emilio visited UIUC in December 2003
• Glaucio visited USP and LNLS (Syncroton Light National Laboratory – Campinas, SP) in April 2004
• Conference papers presented at FGM2004 and ICTAM2004
• The following journal paper is at final stage: “Topology Optimization Applied to the Design of Functionally Graded Material (FGM) Structures”
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Homogenization for FGM Materials

These materials possess continuously graded properties with gradual change in microstructure;

Calculation of effective properties is very difficult using analytical methods

Homogenization method can be applied

FGM Composite material example
To solve homogenization equations the graded finite element (Kim and Paulino 2002) is used which considers a continuous distribution of material inside unit cell.

\[ E(x) = \sum_{I=1}^{nnodes} E_I N_I(x) \]

- \( E \): material property
- \( E_I \): material property evaluated at FEM nodes
- \( x=(x, y) \): position
- Cartesian coordinates

Diagram: Homogenization for FGM Materials
Material properties:

- **Elastic properties**
  - \( E_1 = 8; E_2 = 1 \)
  - \( \nu_1 = \nu_2 = 0.3 \)
  - \( \alpha_1 = 1; \alpha_2 = 2 \)
  - \( H = \beta E \alpha \)

- **Thermoelastic properties**

FGM law:

\[
E = \left( (E_1 - E_2) \cos 2\pi x' + E_1 + E_2 \right) / 2
\]

\[
\beta = \left( (\beta_1 - \beta_2) \cos 2\pi x' + \beta_1 + \beta_2 \right) / 2
\]

Homogenized properties:

\[
E^H = \begin{bmatrix} 3.68 & 1.1 & 0. \\ 1.1 & 4.83 & 0. \\ 0. & 0. & 1.29 \end{bmatrix}; \quad \beta^H = \begin{bmatrix} 5.73 \\ 6.72 \\ 0. \end{bmatrix}
\]
Axyssimetric composite (Application to bamboo and natural fiber composites)

Elastic properties:

\[ E_1 = 10; \quad E_2 = 2.1; \]
\[ \nu_1 = \nu_2 = 0.3 \]

FGM law:

\[ \mathbf{E} = \left( (E_1 - E_2) \cos 2\pi r' + E_1 + E_2 \right) / 2 \]

Homogenized properties

\[
E^H = \begin{bmatrix}
5.39 & 2.01 & 1.62 & 0. \\
2.01 & 5.85 & 1.65 & 0. \\
1.62 & 1.65 & 6.49 & 0. \\
0. & 0. & 0. & 1.89
\end{bmatrix}
\]
Material Design - Introduction

Homogenization method can be combined with optimization algorithms to design composite materials with desired performance.

Specify the desired Material properties  Design the Composite Material

Inverse Problem (Synthesis)

How to implement it??
Consider the periodic composite:

Effective Properties ("equivalent" homogeneous medium)

Depend on unit cell topology

Change effective properties !!

Changing unit cell topology
Material Design Method

Calculation of Effective properties \rightarrow \text{Homogenization Method} \rightarrow \text{Topology Optimization} \rightarrow \\
Design in a mesoscopic scale rather than a microscopic scale (Physics approach)
Material Design Method

- Design of negative Poisson’s ratio materials
  (Bendsoe 1989, Sigmund 1994, Fonseca 1997)
- Design of thermoelastic materials
  (Sigmund and Torquato 1996, Chen and Kikuchi 2001)
- Design of Piezocomposite materials
  (Silva and Kikuchi 1998)
- Design of Band-Gap materials
  (Sigmund and Jensen 2002)

How to build them?
- Rapid Prototyping Techniques
- Microfabrication technique (described ahead)
Topology Optimization Concept

It combines FEM with optimization algorithms to find the optimum material distribution inside of a fixed design domain.

It turns the design process more generic and systematic, and independent of engineer previous knowledge. Largely applied to automotive and aeronautic industries to design optimized parts. In addition, has been applied to:

- Design of compliant mechanisms;
- Design of piezoelectric actuators;
- Design of “MEMS”;
- Design of electromagnetic devices;
- Design of composite materials
Topology Optimization Concept

Optimum topology
Topology Optimization Concept

Based on two main concepts:

• Extended Fixed Domain

• Relaxation of the Design Variable
Old approach: Find the boundaries of the unknown structure (Zienkiewicz and Campbell 1973)

New approach: Find the material distribution in the extended fixed domain (Bendsøe and Kikuchi 1988)
The material model formulation for intermediate materials defines the level of problem relaxation. The use of discrete values will cause numerical instabilities due to multiple local minimum. Thus, the material must assume intermediate property values during the optimization mixture law or material model.

The material model formulation for intermediate materials defines the level of problem relaxation.
Relaxation of the Design Problem

Material Model: Density Method

\[ E_{ijkl}^p = x^p E_{ijkl}^0 \]

property

fraction of material in each point

A point with material

A point with no material

\( \Omega \)

Structure Design Domain
In each finite element $n$ property $c_n$ is given by:

$$c_n = x_n^p c_0;$$

$c_0$ : property of basic material

End of Optimization:

- $x_n = x_{low}$ $\Rightarrow$ element is “air”
- $x_n = 1$ $\Rightarrow$ element is full of material
Maximize: $F(x)$, where $x=[x_1,x_2,\ldots,x_n,\ldots,x_{NDV}]$ subject to:

$$c_{ijkl} \geq c_{\text{low}}, \; i, j, k, l \text{ are specified values}$$

$$0 < x_{\text{low}} \leq x_n \leq 1$$

$$W = \sum_{n=1}^{NDV} x_n^p V_n > W_{\text{low}}$$

symmetry conditions

$F(x)$ - function of effective properties

$x$ - design variables

$W$ - constraint to reduce intermediate densities

($V_n$ - volume of each element)
Example

- Plane Stress
- Isotropic
- Poisson’s ratio = -0.5

(Fonseca 1997)

Unit Cell

Composite Material
Example

- Orthotropic
- Two negative and one positive Poisson’s ratio

(Fonseca 1997)
Thermoelastic Composites

(negative thermal expansion)  (negative thermal expansion)

(high positive thermal expansion)  (zero thermal expansion)

(Sigmund & Torquato 1996)
Example

2D Piezocomposite Unit Cell (hydrophone)

Initially

Optimized Microstructure

Piezocomposite

Improvement in relation to the 2-2 piezocomposite unit cell:

|d_h|: 3. times

d_h g_h: 9.22 times

k_h: 3.6 times

stiffness constraint: c^{E}_{33}>1.10^{10}N/m^2
Composite Manufacturing

Microfabrication by coextrusion technique

Theoretical unit cell

Crumm and Halloran (1997)

SEM Image

250 μm

Fugitive

Ceramic

Feedrod

Reduction Zone

Extrudate

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Experimental Verification

<table>
<thead>
<tr>
<th></th>
<th>Measured Performances</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(d_h(pC/N))</td>
<td>(d_h g_h(fPa^{-1}))</td>
<td></td>
</tr>
<tr>
<td>Solid PZT</td>
<td>68.</td>
<td>220.</td>
<td></td>
</tr>
<tr>
<td>Optimized</td>
<td>308. (257.)</td>
<td>18400. (19000.)</td>
<td></td>
</tr>
</tbody>
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Theoretical

Prototype
3D Piezocomposite Unit Cell (hydrophone)

Poled in the $z$ direction

Improvement in relation to the reference unit cells:

| $|d_h|$ | 5 times |
| $d_h g_h$ | 45 times |
| $k_h$ | 3.71 times |

stiffness constraint: $c_{zz}^E > 4.10^9 \text{N/m}^2$
Composite Manufacturing

Rapid Prototyping: Stereolithography Technique
3D prototypes
Recent works in the Field

- Fujii et al. 2001 - Design of 2D thermoelastic microstructures;
- Torquato et al. 2003 - Design of 3D composite with multifunctional characteristics;
- Guedes et al. 2003 - Energy bounds for two-phase composites
- Diaz and Bénard 2003 - Material Design using polygonal cells
The results presented give us an idea about the potentiality of applying homogenization and optimization methods to model and design composite materials. However, synthesis methods for designing these materials are still in the beginning, and the performance limits of advanced composite materials can be improved more;

Design of FGM materials using topology optimization will allow us to explore the potential of FGM concept;

As a future trend, the design of composite materials considering nanoscale unit cells started been studied by some scientists.
Theoretical Formulation

Homogenization Procedure

- Strains are expanded as a global function plus a local oscillation proportional to the global strain;
- The unit cell response (microscopic strain) is obtained considering independent load cases (unit strains) under periodic boundary conditions;
- The microscopic strains are integrated to obtain composite “average” properties;
- After a global analysis, the strains inside the cell can be obtained by using the localization functions;