Abstract: In this talk we shall discuss algorithms and CAD tools for the design and analysis of structures for high performance applications using advanced composite materials. An extensive mathematical theory for optimal structural (e.g., shape) design has been developed over the past thirty years. Aspects of this theory have been used in the design of components for hypersonic vehicles and thermal diffusion systems based on homogeneous materials. Enhancement of the design methods to include optimization of the microstructure of the component is a significant innovation which can lead to major enhancements in component performance. Our work is focused on the adaptation of existing theories of optimal structural design, e.g., optimal shape design, to treat the design of structures using advanced composite materials, e.g., fiber reinforced, resin matrix materials. In this talk we shall discuss models and algorithms for the design of simple structures from composite materials, focusing on a problem in thermal management. We shall also discuss methods for the integration of active structural controls into the design process.

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**Problem:** Integrated design of structures, their materials, and embedded active controls

**Issues:**

1. **Shape optimization**

2. Material analysis and design

3. Actuator design and placement

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**Shape Design:** Find shape of an object to optimize a design criterion and satisfy design constraints.

**Abstract Formulation:**

- $\Omega \subset \mathbb{R}^n$ the object shape

- $A(u, \Omega) = 0$ defines $u(z) \in \mathbb{R}^m$, $z \in \Omega$

- Given $f(u, \Omega)$ a real-valued function

**Optimal Shape Design Problem:**

$$\min_{\Omega \in \mathcal{O}} \{ f(u, \Omega), \, A(u, \Omega) = 0 \}$$
Two essential problems:

1. Select the topology for the structure (cylindrical, rectangular, etc.); and

2. Within the designated topology find the best shape.

Remarks:

- The first problem is very difficult; e.g., introduction of internal holes in a structure to reduce the weight without violating design constraints.

- The second problem (initial and final topologies are the same) can usually be treated by gradient methods.

Example: Optimal Compliance Design of an Elastic Structure

Problem: Design an elastic structure containing a large number of "cells" in a continuous array; e.g., fiber reinforced structure.

Remark: If the array is locally periodic, the macroscopic moduli may be computed using homogenization theory.

Design Parameters: dimensions \((a, b)\) and orientation \(\theta\) of the microscopic elements.
Design Parameters

Design Algorithm:

1. Use homogenization to compute the local effective elasticity tensor $E^H(x, (a, b, c, \theta))$.

2. Compute gradient of performance function

3. Steepest descent on design parameters
Effective Parameter Model:

"Effective" elasticity tensor $E^H(x)$ may be computed using homogenization theory.

1. Solve cell problem

$$
\sum_{i,j,m,n=1}^{2} \int_Y E_{ijmn} \frac{\partial \chi_m^{(kt)}}{\partial y_n} \frac{\partial \nu_i}{\partial y_j} dY = \\
\sum_{i,j,m,n=1}^{2} \int_Y E_{ijmn} \frac{\partial \nu_i}{\partial y_j} dY
$$

for the characteristic deformation $\chi_m^{(kt)}$

2. Compute the homogenized elasticity tensor

$$
E_{ijkt}^H = \sum_{m,n=1}^{2} \int_Y \left( E_{ijkt} - E_{ijmn} \frac{\partial \chi_m^{(kt)}}{\partial y_n} \right) dY
$$
Displacement Model: Assume smooth variation across structure.

\[ E^{H,(a,b,\theta)}_{ijkl}(x) = \sum_{IJKL=1}^{2} E^{H}_{IJKL} R_{ij}(\theta(x)) \]

\[ R_{jI}(\theta(x)) R_{kK}(\theta(x)) R_{Ll}(\theta(x)) \]

\[ R(\theta(x)) = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \]

is the (local) rotation matrix.

Macroscopic Behavior: (For each \( \Theta = (a, b, \theta) \))

\[ \sum_{i,j,k,l=1}^{2} \int_{\Omega} E^{H,\Theta}_{ijkl}(x) \frac{\partial u_{k}}{\partial x_{i}} \frac{\partial u_{l}}{\partial x_{j}} d\Omega \]

\[ = \sum_{i=1}^{2} \int_{\Omega} f_{i} \nu_{i} d\Omega + \sum_{i=1}^{2} \int_{\Gamma} \tau_{i} \nu_{i} d\Gamma \]

\( f_{i}, i = 1, 2 \) are the applied body forces in \( \Omega \),
\( \tau_{j}, j = 1, 2 \) are the tractions applied on the boundary \( \Gamma_{r} \subset \Gamma = \partial \Omega \).
Optimal Compliance Design

\[
\min_{\{\Theta=(a,b,\rho)\}} \sum_{ijkl=1}^{2} \int_{\Omega} E_{ijkl}(x) \frac{\partial \nu_k \partial \nu_i}{\partial x_l \partial x_j} d\Omega
\]
subject to the constraint (*) and
\[
\int_{\Omega} (1 - a(x)b(x)) d\Omega \leq |\Omega_F|
\]
\(\Omega_F\) = the maximum volume fraction allocated to the reinforcing material.

Using a penalty method, the optimization problem is approximated by

\[
\max \min_{\Theta, \nu \in V} \Pi^f(\nu)
\]
where \(\Pi^f(\nu)\) is the total potential energy

\[
\Pi^f(\nu) = \frac{1}{2} \sum_{ijkl=1}^{2} \int_{\Omega} E_{ijkl}(x) \frac{\partial \nu_k \partial \nu_i}{\partial x_l \partial x_j} d\Omega
\]
\[
+ \frac{1}{2} \sum_{i=1}^{2} \int_{\Gamma_D} \frac{1}{2}(\nu_i - g_i)^2 d\Gamma
\]
\[
- \sum_{i=1}^{2} \int_{\Omega} f_i \nu_i d\Omega - \sum_{i=1}^{2} \int_{\Gamma_R} \tau_i \nu_i d\Gamma
\]
Introduce the Lagrangian

\[ \mathcal{L} = \Pi^i - \lambda \int_{\Omega} (1 - ab) d\Omega - \Omega_F \]
where \( \lambda \leq 0 \) is a Lagrange multiplier.

Taking the variation of \( \mathcal{L} \) with respect to \( u \) and the design variables \( \Theta = (a, b, \theta) \) gives the optimality conditions:

\[ \int_{\Omega} \sum_{ijkl=1}^{2} \frac{1}{2} \left[ \frac{\partial E_{ijkl}^{\Theta}}{\partial a_{jk}} \frac{\partial u_k}{\partial x_l} + \lambda b \right] \delta \omega \geq 0 \]

\( \forall \delta a = a^* - a, \ 0 < a^* < 1 \in \Omega \)

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Optimality conditions:

\[ a = \min \left\{ \max \left[ 0, a - \rho_a \left( \frac{1}{2} \frac{\partial E_{ijkl}^{\Theta}}{\partial a_{jk}} \frac{\partial u_k}{\partial x_l} + \lambda b \right), 1 \right] \right\} \]

\[ b = \min \left\{ \max \left[ 0, b - \rho_b \left( \frac{1}{2} \frac{\partial E_{ijkl}^{\Theta}}{\partial b} \frac{\partial u_k}{\partial x_l} + \lambda a \right), 1 \right] \right\} \]

\[ \lambda = \min \left\{ 0, \lambda - \rho_\lambda \left( \int_{\Omega} (1 - ab) d\Omega - \Omega_F \right) \right\} \]

\[ \frac{1}{2} \frac{\partial E_{ijkl}^{\Theta}}{\partial \theta} \frac{\partial u_k}{\partial x_l} \frac{\partial u_i}{\partial x_j} = 0 \]

for arbitrary positive numbers \( \rho_a, \rho_b, \rho_\lambda \)
Example: Optimal design of a thermal diffuser using composites

Problem: Select the shape $\Omega$ of the diffuser and the parameterization $\Theta$ of $\Omega_f$ (volume fraction, orientation, packing, etc.) of the material infrastructure to minimize the weight of the diffuser and meet operational objectives.

(i) the maximum temperature at the payload-diffuser interface must not exceed $T_m$;

(ii) no part of the diffuser can be thinner than some constant $d$; and

(iii) for convective cooling, the flux on the transmission interface of the diffuser must be below $q_m$. 

Composite Material Thermal Diffuser
Model:

Assume: Conductivity of the fiber material is \( k \), conductivity of the matrix material is \( K \) (could be anisotropic)

Conductivity tensor: \( \{a_{ij}^{(z,y,z)}, i,j = 1,2,3\} \)

\[
\frac{\partial}{\partial x_i} \left( a_{ij}^{(z)} \frac{\partial T^{(z)}}{\partial x_j} \right) = 0
\]

with the boundary conditions

\[
\frac{\partial T^{(z)}}{\partial \eta^{(z)}} = q_{in} \text{ on } \Sigma_1; \quad \frac{\partial T^{(z)}}{\partial \eta^{(z)}} = 0 \text{ on } \Sigma_2
\]

\[
\frac{\partial T^{(z)}}{\partial \eta^{(z)}} + \kappa(T^{(z)})p = q_s \text{ on } \Sigma_3
\]

\( \eta/\partial \eta^{(z)} \) is the conormal derivative at the surface.

Design Parameters: \( \Theta \), the fiber orientation and packing, and \( R(z), 0 \leq z \leq L \) the curve defining the shape of the boundary, and \( L \).

Performance Index: Mass of diffuser

\[
\Pi(\Theta, R(\cdot), L) = \int_0^L \int_0^L \rho^{(z,y,z)} R(z)^2 \, dy \, dz
\]

\( \rho^{(z,y,z)} \) is the mass density in a cross section \( C(z) \).

The optimal design problem is

\[
\min_{\Theta, R(\cdot), L} \Pi(\Theta, R(\cdot), L)
\]
Homogenization: (local)

**Effective Conductivity:**

\[ \alpha_{ij} = M(a_{ij}) - M \left( \sum_k a_{ik} \frac{\partial \chi^k}{\partial y_k} \right) \]

**Macroscopic Behavior:**

\[ \Delta A u = -\alpha_{ij} \frac{\partial^2 u^0}{\partial x_i \partial x_j} = f \]

"Corrector:"

\[ - \frac{\partial}{\partial y_i} \left( a_{ij}(y) \frac{\partial \chi^i}{\partial y_j} \right) = - \frac{\partial a_{ij}(y)}{\partial y_i} \]

**Optimal Design:**

*Adjoin constraints to performance function:*

\[ \Pi_{\mu}(\Theta, R(\cdot), L(\nu)) = \Pi(\Theta, R(\cdot), L) \]

\[ + \frac{1}{2} \sum_{i, j=1}^{2} a_{ij}(x) \frac{\partial \nu}{\partial x_i} \frac{\partial \nu}{\partial x_j} + \int_{\Omega} f \nu d\Omega \]

\[ + \frac{1}{2} \sum_{i, j=1}^{2} \left( \frac{1}{\mu} \int_{\Gamma} (\nu - g)^2 d\Gamma \right) \]

\( \mu > 0 \) is a small parameter.
Define the Lagrangian:

\[ \mathcal{L}(\nu, \Theta, R(\cdot), L, \Lambda) = \Pi_\mu(\nu) \]

\[ -\Lambda \left[ \int_{\Omega_F} \rho_F dz dy dz - M_F \right] \]

Lagrange multiplier \( \Lambda \leq 0 \).

**Optimality Criteria:**

Obtained from variation of \( \mathcal{L} \) with respect to state \( u \) and design variables \( (\Theta, R(\cdot), L) \).