AE 760AA: Micromechanics and multiscale modeling

Lecture 6 - Orientation Averaging

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February 11, 2019

schedule

- Feb 11 - Orientation Averaging
- Feb 13 - Physical measurements (HW2 Due)
- Feb 18 - Variational Calculus
- Feb 20 - Variational Calculus

outline

- orientation averaging
- closure approximations
- variational calculus

orientation average

orientation tensor

- Within a given volume, a distribution of fibers can be defined by some orientation distribution function, $\psi(\theta, \phi)$.
- Advani and Tucker introduced tensor representations of fiber orientation distribution functions

$$a_{ij} = \oint p_i p_j \psi(p) dp$$

- And

$$a_{ijkl} = \oint p_i p_j p_k p_l \psi(p) dp$$

- Note: any order tensor may be defined in this manner, the orientation distribution function must be even, due to fiber symmetry, and thus any odd-ordered tensor will be zero.

orientation averaging

- Consider $T(p)$ to be some tensor property of a material, as a function of material orientation
- The orientation average of $T(p)$ is denoted by angle brackets and is given by
  $\langle T \rangle = \oint T(p)\psi(p)dp$
- For a uni-directional fiber, we would expect $\langle T \rangle$ to be transversely isotropic, which for a second-order tensor requires
  $\langle T_{ij} \rangle = A_1 \langle p_i p_j \rangle + A_2 \delta_{ij}$
- but $\langle p_i p_j \rangle$ is the second-order orientation tensor
- The unknown constants, A_1 and A_2, can be easily solved for in terms of the uni-directional properties

orientation averaging

- Similarly, if T is a fourth-order tensor property then transverse isotropy requires that
  $$\langle T_{ijkl} \rangle = B_1 a_{ijkl} + B_2(a_{ij}\delta_{kl} + a_{kl}\delta_{ij}) + B_3(a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}) + B_4(\delta_{ij}\delta_{kl}) + B_5(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$
- We can solve for B_α by considering fibers aligned in the three-direction, we have $a_{3333} = 1$ and all other $a_{ijkl} = 0$.
- We can choose any values of i, j, k, l that would give 5 unique equations to solve equations for B_α

orientation averaging

- Here we will consider T_{1111}, T_{3333}, T_{1122}, T_{2233}, T_{1313}.

$$T_{1111} = B_4 + 2B_5$$
$$T_{3333} = B_1 + 2B_2 + 4B_3 + B_4 + 2B_5$$
$$T_{1122} = B_4$$
$$T_{2233} = B_2 + B_4$$
$$T_{1313} = B_3 + B_5$$

orientation averaging

- After some manipulation, we find

$$
\begin{aligned}
B_1 &= T_{1111} + T_{3333} - 2T_{2233} - 4T_{1313} \\
B_2 &= T_{2233} - T_{1122} \\
B_3 &= T_{1313} - \frac{1}{2}(T_{1111} - T_{1122}) \\
B_4 &= T_{1122} \\
B_5 &= \frac{1}{2}(T_{1111} - T_{1122})
\end{aligned}
$$

closure approximations

closure approximations

- While theoretically any-order orientation tensor is possible, in practice only the second-order tensor is used
- Microscopic measurements do not give enough information for higher-order tensors to be useful
- Software simulations have not implemented the fourth-order tensor
- To predict stiffness, we need the fourth-order tensor
- Closure Approximations are a way to approximate the fourth-order tensor from the second-order tensor

linear closure approximate

- For 3D orientations, the linear approximation is given by
$$a_4^l = -\frac{1}{35}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) +$$
$$\frac{1}{7}(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{kl}\delta_{ij} + a_{jl}\delta_{ik} + a_{jk}\delta_{il})$$
- For planar orientations we simply replace the two coefficients with $-\frac{1}{24}$ and $\frac{1}{6}$

quadratic closure

- We can also use a quadratic closure method $a_4{}^q = a_{ij}a_{kl}$
- If the fibers are randomly aligned, the linear closure will give the exact result
- If the fibers are perfectly oriented, the quadratic closure will give the exact result

hybrid closure

- Advani proposed a hybrid closure to take advantage of both the linear and quadratic methods
- We will introduce a parameter f and use it to combine both linear and quadratic closures

$$a_4{}^h = (1 - f)a_4{}^l + fa_4{}^q$$

- Ideally, we would like f to be 1 for perfectly oriented fibers and 0 for random fibers
- Advani proposes $f = Aa_{ij}a_{ji} - B$
- Where $A = 3/2$ and $B = 1/2$ for 3D orientations and $A = 2$ and $B = 1$ for planar orientation

orthotropic fitted closure

- A more recent method that is commonly used is known as the orthotropic fitted closure
- The fourth-order tensor is approximated in the principal direction, then rotated back out if necessary
- In the principal direction, the fourth-order tensor will be orthotropic (represented in 6x6 as)

$$A_4 = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 & 0 \\ A_{12} & A_{22} & A_{23} & 0 & 0 & 0 \\ A_{13} & A_{23} & A_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & A_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & A_{66} \end{bmatrix}$$

orthotropic fitted closure

- The symmetry of the orientation tensor requires that A_{66} (which is a_{1212}) be equal to A_{12} (which is a_{1122}).
- By the same symmetry, we have $A_{55} = A_{13}$ and $A_{44} = A_{23}$.
- We also know that $a_{ijkk} = a_{ij}$, which imposes the following equations:

$$\begin{aligned}
A_{11} + A_{66} + A_{55} &= a_{11} \\
A_{66} + A_{22} + A_{44} &= a_{22} \\
A_{55} + A_{44} + A_{33} &= a_{33}
\end{aligned}$$

orthotropic fitted closure

- This leaves only three independent variables in the fourth-order tensor that need to be found.
- Different authors have proposed different functions to fit these three independent variables
- They are fit to give the best mold simulation predictions, but do not necessarily have any physical application

discrete calculations

- To compare with our laminate analogy we can calculate the orientation tensor for discrete orientation states
  $$a_{ij} = \frac{1}{N} \sum p_i p_j$$
  for second-order tensors and
  $$a_{ijkl} = \frac{1}{N} \sum p_i p_j p_k p_l$$

example

- Compare Mori-Tanaka stiffness predictions for direct calculation and orientation averaging
- Compare $[0/90]_S$, $[\pm 45]_S$, and $[0/\pm 45/90]_S$
- **link**
- Also compare the results with a closure approximation of the fourth-order tensor

variational calculus

differential and variational statements

- A differential statement includes a set of governing differential equations established inside a domain and a set of boundary conditions to be satisfied along the boundaries
- A variational statement is to find stationary conditions for an integral with unknown functions in the integrand
- Variational statements are advantageous in the following aspects
  - Clear physical meaning, invariant to coordinate system
  - Can provide more realistic descriptions than differential statements (concentrated loads)
  - More easily suited to solving problems numerically or approximately
  - Can be more systematic and consistent than building a set of differential equations

stationary problems

- If the function $F(u_1)$ is defined on a domain, then at $\frac{dF}{du_1} = 1$ it is considered to be stationary
- This stationary point could be a minimum, maximum, or saddle point
- We use the second derivative to determine which of these it is: >0 for a minimum, <0 for a maximum and =0 for a saddle point
- For a function of n variables, $F(u_n)$ the stationary points are
  $$\frac{\partial F}{\partial u_i} = 0$$
  for all values of i
- and to determine the type of stationary point we use
  $$\sum_{i,j=1,n} \frac{\partial^2 F}{\partial u_i \partial u_j}$$

lagrange multipliers

- Let us now consider a function of several variables, but the variables are subject to a constraint

$$f(u_1, u_2, \ldots)=0$$

- Algebraically, we could use each provided constraint equation to reduce the number of variables
- For large problems, it can be cumbersome or impossible to eliminate some variables
- The Lagrange Multiplier method is an alternative, systematic approach

lagrange multiplier

- For a constrained problem at a stationary point we will have
$$dF = \frac{\partial F}{\partial u_1} du_1 + \ldots + \frac{\partial F}{\partial u_n} du_n = 0$$
- The relationship between du_i can be found by differentiating the constraint
$$df = \frac{\partial f}{\partial u_1} du_1 + \ldots + \frac{\partial f}{\partial u_n} du_n = 0$$
- We can combine these two equations using a Lagrange Multiplier
$$\frac{\partial F}{\partial u_1} du_1 + \ldots + \frac{\partial F}{\partial u_n} du_n + \lambda \left[\frac{\partial f}{\partial u_1} du_1 + \ldots + \frac{\partial f}{\partial u_n} du_n \right]$$
- We can re-group terms as
$$\sum_{i=1}^{n} \left[\frac{\partial F}{\partial u_i} + \lambda \frac{\partial f}{\partial u_i} \right] du_i = 0$$

lagrange multiplier

- The Lagrange Multiplier, λ is an arbitrary function of u_i
- We can choose the Lagrange Multiplier such that
$$\frac{\partial F}{\partial u_n} + \lambda \frac{\partial f}{\partial u_n} = 0$$
- Which now leaves
$$\frac{\partial F}{\partial u_i} + \lambda \frac{\partial f}{\partial u_i} = 0 \qquad i = 1, 2, \ldots, n-1$$
- We now define a new function $F^* = F + \lambda f$

lagrange multiplier

- This converts a constrained problem in n variables to an unconstrained problem in $n + 1$ variables
- Notice that while the stationary values of F^* will be the same as the stationary values to F, they will not necessarily correspond
- For example, a minimum in F^* might be a maximum in F
- This provides a systematic method for solving problems with any number of variables and constraints, and is also well-posed for numeric solutions

example

- Design a box with given surface area such that the volume is maximized
- The box has no cover along one of the surfaces (open-face box)
- This gives the surface area as $A = xy + 2\,yz + 2\,xz = C$
- **worked example**