AE 760AA: Micromechanics and multiscale modeling

Lecture 12 - Hashin-Shtrikman Bounds

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schedule

- Mar 25 - Hashin-Shtrickman bounds
- Mar 27 - Periodic Boundary Conditions
- Apr 1 - Fourier Analysis
- Apr 3 - Method of Cells

outline

- hashin-shtrikman
- boundary conditions

hashin-shtrikman

bounds

- We consider the Voigt and Reuss micromechanics models as bounding cases, properties should need exceed the limits of these two cases
- Hashin and Shtrikman used variational principles to define more rigorous bounds for composite properties
- They did this by comparing a heterogeneous composite RVE with an equivalent homogeneous RVE

heterogeneous

$$\sigma_{ij,j} = 0$$
$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

$$U = \frac{1}{2}C_{ijkl}\epsilon_{ij}\epsilon_{kl}$$

homogeneous

$$\sigma^{(0)}_{ij,j} = 0$$

$$\sigma^{(0)}_{ij} = C^{(0)}_{ijkl}\epsilon^{(0)}_{kl}$$

$$U = \frac{1}{2}C^{(0)}_{ijkl}\epsilon^{(0)}_{ij}\epsilon^{(0)}_{kl}$$

relation

- To relate the two boundary problems, we introduce the following

$$
\begin{aligned}
u_i &= u_i^{(0)} + u_i^d \\
\epsilon_{ij} &= \epsilon_{ij}^{(0)} + \epsilon_{ij}^d \\
\sigma_{ij} &= p_{ij} + C_{ijkl}^{(0)}\epsilon_{kl} = p_{ij} + C_{ijkl}^{(0)}(\epsilon_{ij}^{(0)} + \epsilon_{ij}^d)
\end{aligned}
$$

- ${u_i}^d$ is the disturbance displacement field and p_{ij} is called the polarization stress

boundary conditions

- One common RVE boundary condition is known as homogeneous displacement
- Under homogeneous displacement boundary conditions we have

$$u_i = \bar{u}_i = u_i^{(0)}$$

along the boundary

- Under this condition we have $u_d = 0$ along the boundary

hashin-shtrikman

- Hashin-Shtrikman then considered the following functional $\Pi = \int_V (C_{ijkl}{}^{(0)} \epsilon_{ij}{}^{(0)} \epsilon_{kl}{}^{(0)} - \Delta C_{ijkl}{}^{-1} p_{ij} p_{kl} + p_{ij} \epsilon_{ij}{}^{d} + 2 p_{ij} \epsilon_{ij}{}^{(0)}) dV$
- Where

$$
\begin{aligned}
\Delta C_{ijkl} &= C_{ijkl} - C_{ijkl}^{(0)} \\
p_{ij} &= \Delta C_{ijkl} \epsilon_{kl} \\
\epsilon_{ij}^{d} &= \epsilon_{ij} - \epsilon_{ij}^{(0)}
\end{aligned}
$$

- This functional corresponds to the strain energy in a composite when the strain field and polarization field are exact solutions

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- We can choose the comparison solid such that $\delta \boldsymbol{Pi}$ will either be a local maximum or a local minimum
- When ΔC is negative definite then the stationary value of the functional is a minimum
- When ΔC is positive definite then the stationary value of the functional is a maximum
- The functional will be stationary when $(C_{ijkl}{}^{(0)}\epsilon_{kl}{}^{d})_{,j} + p_{ij,j} = 0$

hashin-shtrikman

- In general, I don’t know how often you will need to use the Hashin-Shtrikman bounds
- For a more complete derivation, see textbook pp. 170-186

boundary conditions

macro and micro fields

- In micromechanics, one of our primary goals is to relate a heterogeneous material to some equivalent homogeneous material
- We call ϵ_{ij} and σ_{ij} the point-wise or microscopic strain and stress
- $\bar{\epsilon}_{ij}$ and $\bar{\sigma}_{ij}$ are the macroscopic strain and stress, and are related by some unknown homogenized stiffness

$$\bar{\sigma}_{ij} = C^*_{ijkl}\bar{\epsilon}_{kl}$$

- In a homogeneous body (or equivalent homogeneous body), $sig\bar{m}a_{ij}$ and $\bar{\epsilon}_{ij}$ will be constant throughout

average stress theorem

- In general the stress field σ_{ij} will not be constant in a heterogeneous body
- If a heterogeneous body is subjected to homogeneous tractions with no body forces such that

$$t_i^0 = \bar{\sigma}_{ij} n_j$$

- And we find that

$$\langle \sigma_{ij} \rangle = \bar{\sigma}_{ij}$$

average strain theorem

- Similarly, in general the strain field, ϵ_{ij} will not be constant in a heterogeneous body
- If a heterogeneous body is subjected to a homogeneous displacement such that

$$u_i^0 = \bar{\epsilon_{ij}} x_j$$

- And we find that

$$\langle \epsilon_{ij} \rangle = \bar{\epsilon}_{ij}$$

hill mandel macrohomogeneity condition

- Hill and Mandel posed the question: Under what conditions will the average strain energy density of a heterogeneous body be equivalent equivalent to a homogeneous body?
- In other words, they wanted show under what conditons

$$\langle \sigma_{ij} \epsilon_{ij} \rangle = \bar{\sigma}_{ij} \bar{\epsilon}_{ij}$$

hill mandel macrohomogeneity

- First we note that

$$\bar{\sigma}_{ij}\bar{\epsilon}_{ij} = \frac{1}{V}\int_V \sigma_{ij}\bar{\epsilon}_{ij}dV = \frac{1}{V}\int_V \bar{\sigma}_{ij}\epsilon_{ij}dV = \frac{1}{V}\int_V \bar{\sigma}_{ij}u_{i,j}dV$$

- Thus we can say that when $\langle\sigma_{ij}\epsilon_{ij}\rangle = \bar{\sigma}_{ij}\bar{\epsilon}_{ij}$

$$\langle\sigma_{ij}\epsilon_{ij}\rangle - \bar{\sigma}_{ij}\bar{\epsilon}_{ij} = \frac{1}{V}\int_V (\sigma_{ij}u_{i,j} - \bar{\sigma}_{ij}u_{i,j} - \sigma_{ij}\bar{\epsilon}_{ij} + \bar{\sigma}_{ij}\bar{\epsilon}_{ij})dV$$

hill mandel macrohomogeneity

- After some algebra and applying the divergence theorem, we can write this as

$$\langle \sigma_{ij}\epsilon_{ij}\rangle - \bar{\sigma}_{ij}\bar{\epsilon}_{ij} = \frac{1}{V}\oint_V n_k(\sigma_{ik} - \bar{\sigma_{ik}})(u_i - x_j\bar{\epsilon}_{ij})dS$$

- The right-hand side can be made to vanish in various ways, but the most common are homogeneous traction, homogeneous displacement, and periodic boundary conditions

finite elements

- There are a few things we need to do when using finite elements
- First, we should ensure the mesh we use is periodic
- Second, we should ensure that our boundary conditions satisfy Hill-Mandel and that our mesh is converged
- Periodic boundary conditions converge more quickly than homogeneous stress or displacement
- Third, we should repeat our periodic structure (2x2, 3x3) to check that the effective stiffness remains constant
- We find homogenized properties by taking the volume-averaged stress and strain