Lecture 12 - Hashin-Shtrikman Bounds

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## schedule

- Mar 18 Hashin-Shtrickman bounds
- Mar 23 Periodic Boundary Conditions
- Mar 25 Fourier Analysis
- Mar 30 Method of Cells

## outline

- hashin-shtrikman
- boundary conditions

# hashin-shtrikman

- 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

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## heterogeneous

$$\begin{split} \sigma_{ij,j} &= 0 \\ \sigma_{ij} &= C_{ijkl} \epsilon_{kl} \\ U &= \frac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl} \end{split}$$

$$\begin{split} \sigma_{ij,j}^{(0)} &= 0 \\ \sigma_{ij}^{(0)} &= C_{ijkl}^{(0)} \epsilon_{kl}^{(0)} \\ U &= \frac{1}{2} C_{ijkl}^{(0)} \epsilon_{ij}^{(0)} \epsilon_{kl}^{(0)} \end{split}$$

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## 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

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

along the boundary

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

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#### 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

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

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

### hashin-shtrikman

- We can choose the comparison solid such that  $\delta\Pi$  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 \( \Delta C \) is positive definite then the stationary value of the functional is a maximum
- The functional will be stationary when

$$\left(C_{ijkl}^{(0)}\epsilon_{kl}^{d}\right)_{,j}+p_{ij,j}=0$$

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#### 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<sub>ij</sub> and σ<sub>ij</sub> the point-wise or microscopic strain and stress
- ē<sub>ij</sub> and σ̄<sub>ij</sub> 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),  $\bar{\sigma}_{ij}$  and  $\bar{\epsilon}_{ij}$  will be constant throughout

## average stress theorem

- In general the stress field σ<sub>ij</sub> 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,  $\epsilon_{ij}$  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

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

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# 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

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

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# hill mandel macrohomogeneity

First we note that

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

ullet 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

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#### 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