Lecture 11 - Boundary Conditions

Dr. Nicholas Smith

Wichita State University, Department of Aerospace Engineering

17 February 2022

schedule

- 22 Feb - Boundary Conditions
- 24 Feb - Project Descriptions (HW 4 Due)
- 1 Mar - FEA In-class
- 3 Mar - SwiftComp (In-class) (HW 5 Due)

outline

- hashin-shtrikman
- boundary conditions

hashin-shtrikman

bounds

- We consider the Voigt and Reuss micromechanics models as bounding cases, properties should never 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

$$u_i = u^{(0)}_i + u^d_i$$
$$\epsilon_{ij} = \epsilon^{(0)}_{ij} + \epsilon^d_{ij}$$
$$\sigma_{ij} = p_{ij} + C^{(0)}_{ijkl}\epsilon_{kl} = p_{ij} + C^{(0)}_{ijkl}(\epsilon^{(0)}_{ij} + \epsilon^d_{ij})$$

- u^d_i 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

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

- 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 ΔC is positive definite then the stationary value of the functional is a maximum
- The functional will be stationary when

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

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), $\bar{\sigma}_{ij}$ 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

periodic boundary conditions

periodic boundary conditions

- We have used the phrase multiple times in this course
- Periodic Boundary Conditions are used in many different fields, and can be implemented in slightly different ways
- Here we will first discuss the equations for periodic boundary conditions in structural mechanics, then discuss how these can be applied

periodic boundary conditions

- If we have a periodic structure, we denote corresponding faces with + and - superscripts
- From equilibrium, we know that the tractions on opposing faces must be equal and opposite

$$t_i^+ = -t_i^-$$

periodic boundary conditions

- The displacement on opposing surfaces will also be equal with

$$\xi_i^+ = \xi_i^-$$

where

$$\xi_i = u_i - \bar{\epsilon_{ij}} x_j$$

convergence

- In general, homogeneous displacement boundary conditions give an upper bound estimate to stiffness properties
- Homogeneous traction boundary conditions give a lower estimate
- They converge to periodic boundary conditions for increasing RVE size

general application

- In finite element software, solutions are derived from displacement
- Thus it is easiest to implement periodic displacement conditions
- Tractions will be automatically satisfied

general application

- We find the stiffness by applying some arbitrary strain in all directions (i.e. $\bar{\epsilon}_{11} = 1$, $\bar{\epsilon}_{22} = 1$, etc.)
- The volume average of stress then corresponds to the appropriate column of the stiffness matrix
- Some finite element software programs have a built-in method for periodic boundary conditions
- When such a method is not built-in, there are various strategies to enforce the boundary condition

ABAQUS implementation

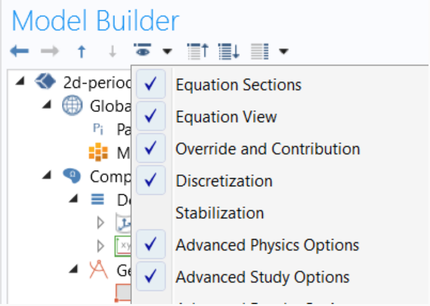
- In ABAQUS PBC's are implemented using equations for each boundary node
- Boundary nodes on a given face are tied to some "dummy" node
- Equations for each node ensure that $\xi_i^+ = \xi_i^-$

COMSOL implementation

- While COMSOL has periodic boundary conditions built-in, there are some quirks to how it is implemented
- The default periodic boundary condition is $u_i^+ = u_i^-$
- This forces displacement to be exactly the same on opposing faces, but we would like for them to be the same with some arbitrary offset
- To implement this requires viewing and modifying the boundary condition equations

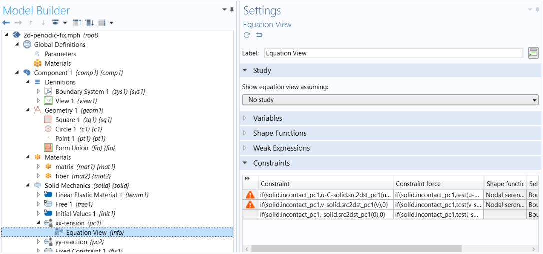
COMSOL implementation

- From the Model Builder on the left-hand side, click the "eye" icon to show the equations



COMSOL implementation

- Next, add a global parameter for the arbitrary strain (in my equations I used ‘C’)
- Now we need to edit the periodic boundary equations in comsol to include an offset of ‘C’
- For example we need to change u-solid.src2dst to u-C-solid.src2dst for the x-faces periodic boundary in COMSOL



shear

- In shear the COMSOL implementation becomes a little bit tricky

$$\xi = u_i - \bar{\epsilon}_{ij} x_j$$

- We need to define displacement on both surfaces under consideration (1 and 2 surface for 12 shear)

rigid constraints

- In general the problem is not constrained against rigid body translation
- Since the displacements are periodic on the surfaces, it is most appropriate to create a point at the center and fix it
- Points can be generated from the geometry menu
- The constraint can be difficult to apply graphically (the point is not visible)
- Instead choose your point from the drop-down

stiffness results

- For any software package, we take the results using the volume-average stiffness and strain
- Recall that in engineering notation we have

$$\sigma_i = C_{ij}\epsilon_j$$

- Before calculating stiffness values, you may want to check that you have a mostly uniform strain
- Stiffness values can be calculated as

$$C_{ij} = \sigma_i/\epsilon_j$$

- Where j is fixed for each load configuration

other comments

- With boundaries under displacement control, we do not need to worry about constraining any other nodes to restrict rigid body motion
- The default (tetrahedral) mesh in COMSOL behaves adequately under these conditions (some small dimpling on the non-restricted surfaces)
- In COMSOL, volume-average properties can be calculated by right-clicking derived values (under results) > average > volume average
- Stress, strain, and stiffness can be found by typing in the "expressions"
- solid.sl11 (Stress Local 11 direction), solid.el11(Strain Local 11 direction)

sample comsol file

- A sample COMSOL file to show the implementation of periodic boundary conditions can be viewed here[1]

[1] http://ndaman.github.io/multiscale/handout/2d-periodic.mph