AE 760AA: Micromechanics and multiscale modeling

Lecture 13 - Periodic Boundary Conditions

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schedule

- Mar 27 - Periodic Boundary Conditions
- Apr 1 - Fourier Analysis
- Apr 3 - Method of Cells
- Apr 8 - Damage Theory

outline

- periodic boundary conditions

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 $t_i^+ = -t_i^-$
- 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 is appropriate for faces where $\bar{\epsilon_{ij}} x_j = 0$
- On faces where $\bar{\epsilon_{ij}} x_j \neq 0$, however, we need to modify the default condition

COMSOL implementation

- To the software, $\xi_i = u_i - \bar{\epsilon_{ij}} x_j$ is all considered u_i
- On boundaries where $\bar{\epsilon_{ij}} x_j \neq 0$, there should be no other source of displacement
- Thus to the software $u_i = \bar{\epsilon_{ij}} x_j$
- On opposing faces, $x_j^+ = -x_j^-$
- This can be implemented in COMSOL using the antiperiodicity requirement
- Some prescribed displacement is then applied in addition to the antiperiodicity requirement, but only on one of the faces

COMSOL implementation

- In some configurations, adjacent faces with continuity and antiperiodicity can create stress concentrations in COMSOL
- This can be resolved by changing the faces to “user-defined”
- Displacements not important to the problem can be ommitted from the condition, and continuity/antiperiodicity constraints enabled only for those faces which concern them

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)
- To avoid stress concentrations, the periodic boundaries are implemented as:
  - antiperiodic in v only on the 1-surface
  - antiperiodic in u only on the 2-surface

shear

- Remember that in all cases the displacement is only applied on one of a pair of faces
- i.e. to apply shear in 12, apply v to one 1-face, and u to one 2-face (the antiperiodicity accounts for the other face)
- In tension/compression the sign does not matter (although tension is typically used)
- In shear the signs must be consistent (check if your 1 and 2 faces chosen for displacement are positive or negative)

rigid constraints

- In shear 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 $\sigma_i = C_{i**j}\epsilon_j$
- 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)