Module 7: Micromechanics
Lecture 28: Homogenization

Introduction

In the previous lectures, we have seen the various micromechanics based approaches to find the effective composite properties. In the standard mechanics approach we introduced the concept of local structure tensor which relates the macroscopic or average strains or stresses in composite to microscopic or local strains or stresses in the phases of composite. In the standard mechanics approach the boundary conditions are chosen such that the applied displacements or tractions produce average strains or stresses in the RVE material.

In this lecture we are going to introduce the concept of homogenization.

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Homogenization

First, we will discuss the key points from statistical homogeneity and standard mechanics approach in the RVE analysis to determine the effective RVE properties. In micromechanical analysis most of the methods accurately predicts the effective composite properties provided that the ratio of the RVE size to the global structural dimension is very small tending to zero. In reference to Figure 7.9, we have $\delta \ll L$. We denote $\frac{\delta}{L} = \eta$.

In the micromechanics based methods the local level and global level analyses are decoupled. The local level analysis considers the microstructural details in its modeling. This analysis gives the effective elastic properties. Further, as we have seen in standard mechanics approach, the local level analysis can also be used to calculate the relationship of the effective or average RVE strain to the local strain within the RVE. However, the global level analysis is used to calculate the effective or the average stress and strain within the equivalent homogenous structure.

The process of calculating effective properties has been termed homogenization by Suquet [1]. Further, the local strains can be estimated from the relationship between average and local strains through local structure tensor obtained from local analysis. This process is called as localization.

In the RVE analysis the RVE is subjected to boundary condition. The solution of this boundary value problem gives the average properties along with the relation between the average and local strains. However, the accuracy of the results depends upon the fact that the applied boundary conditions should be able to reflect the in-situ (or the actual) boundary conditions to which an RVE is subjected. This is explained in the following paragraph.

Consider that the applied boundary conditions to the RVE which produce the same average strain in RVE are not same as the in-situ boundary conditions. Using the principle of minimum of strain energy the average stiffness predicted by the RVE analysis with assumed boundary conditions will be higher than that with in-situ boundary conditions. This is because the in-situ boundary conditions will minimize the strain energy. On the contrary, although the assumed boundary conditions are admissible they produce higher strain energy as the average stress produced is higher. Similarly, for the applied tractions by the principle of minimum of complementary energy the RVE analysis with applied homogeneous boundary produces higher complementary energy than that with in-situ boundary conditions. The applied boundary conditions would produce higher average stress in RVE than due to in-situ boundary conditions and also results in higher compliance. Thus, the RVE analyses with applied displacement boundary conditions give upper bound on effective stiffness whereas applied traction boundary conditions give the lower bound.

The homogenization theory is developed from studies of partial differential equations with rapidly varying coefficients. This theory is based on the two assumptions: the first one is that the fields vary on multiple scales due to existence of a microstructure and second one is that the microstructure is spatially periodic.

In the composite, it is well known to us that the microstructure is spatially periodic. Now in the following we explain that the displacement field is oscillating around the mean displacement and strain field is periodic over this microstructure. Further, the displacement and strain fields are varying over the two length scales.

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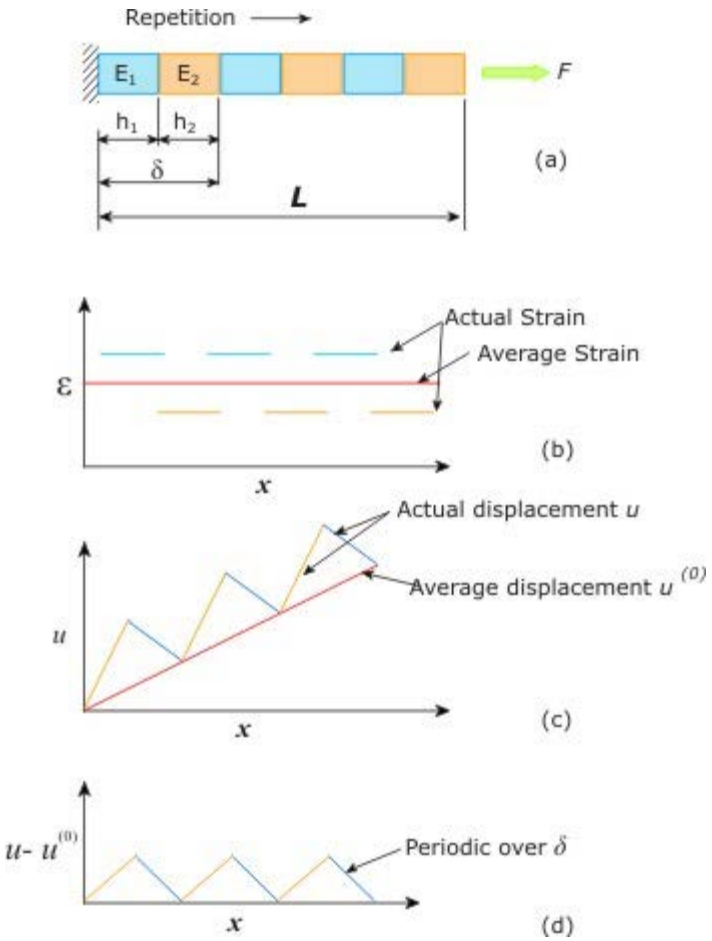

Figure 7.9: (a) A bar representing alternate fibre and matrix (b) actual and average strain (c) actual and average displacement and (d) periodic nature of displacement difference over RVE length

Consider Figure 7.9. Figure 7.9 (a) represents a bar with alternating materials. This bar represents alternate arrangement of fibre and matrix material in cross section. Let δ be the RVE length such that $\delta \ll L$. Figure 7.9 (b) shows the variation of strain field. It should be noted that the strain in either of the element is constant and periodic in nature. However, the average strain in the bar is constant. Figure 7.9(c) shows the variation of actual displacement u and average displacement field $u^{(0)}$. From this figure it is clear that the actual displacement is oscillating around the average displacement. Figure 7.9 (d) shows the variation of $u - u^{(0)}$ and one can easily notice that this variation is periodic over the RVE length. Thus, displacement and strain fields are varying over the two length scales, that is, at micro and macro scales. Further, the strain field and $u - u^{(0)}$ are periodic over the RVE. Thus, the problem of determining effective stiffness can be addressed by using the homogenization concept. The details of theory can be seen in [1-3].

In the following we explain the theory of homogenization in brief.

Let x_i denote the global level or macro coordinates and y_i denote the micro level coordinates. These two level coordinates are related through

$$y_i = \frac{x_i}{\eta} \qquad (7.128)$$

Here η is the ratio of the RVE size to the size of the macroscopic region in which it exists. The field variables involved in this study are approximated by an asymptotic expansion as

$$u_i^{\eta}(x_i, y_i) = u_{0i}(x_i, y_i) + \eta u_{1i}(x_i, y_i) + \eta^2 u_{2i}(x_i, y_i) + \cdots \qquad (7.129)$$

where u_i^{η} is the exact value of the field variable, u_{0i} is the macroscopic or average value of the field variable. In elasticity theory, this is known as continuum level displacement field. The displacements u_{1i}, u_{2i} etc. are the perturbations in the field variable due to the microstructure. These are also called microstructural displacements.

Now, using the small deformations the strain tensor is written as

$$\varepsilon_{ij}(\mathrm{u}) = \frac{1}{2}\left(\frac{\partial u_i^{\eta}}{\partial x_j} + \frac{\partial u_j^{\eta}}{\partial x_i}\right) = \frac{1}{2}\left[\left(\frac{\partial u_{0i}}{\partial x_j} + \frac{\partial u_{0j}}{\partial x_i}\right) + \left(\frac{\partial u_{1i}}{\partial y_j} + \frac{\partial u_{1j}}{\partial y_i}\right) + \eta\left(\frac{\partial u_{1i}}{\partial x_j} + \frac{\partial u_{1j}}{\partial x_i}\right)\right] + h.o.t. \qquad (7.130)$$

In this derivation, the derivative of any function $f^{\eta}(x) = f\left(x, y = \frac{x}{\eta}\right)$ is given using chain rule as

$$\frac{\partial f^{\eta}}{\partial x_i} = \frac{\partial f}{\partial x_i} + \frac{1}{\eta}\frac{\partial f}{\partial y_i} \qquad (7.131)$$

has been used.

Note: The perturbation part of the solution is small, but clearly the corresponding strain is not. This strain is of the same order as the average strain.

Note: The quantities on the local level like stress vary $\frac{1}{\eta}$ times more rapidly than the corresponding global level quantities.

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Equation (7.130) can be simplified neglecting the terms of $o(\eta)$ and higher order. Further, from Equation (7.131) we define the following strain tensors as

$$\varepsilon_{ij} = \bar{\varepsilon}_{ij} + \varepsilon^*_{ij}, \bar{\varepsilon}_{ij} = \frac{1}{2}\left(\frac{\partial u_{0i}}{\partial x_j} + \frac{\partial u_{0j}}{\partial x_i}\right), \varepsilon^*_{ij} = \frac{1}{2}\left(\frac{\partial u_{1i}}{\partial y_j} + \frac{\partial u_{1j}}{\partial y_i}\right) \quad (7.132)$$

where ε_{ij}, as defined earlier, is the local or microstructural strain tensor, $\bar{\varepsilon}_{ij}$ is the average or macroscopic strain tensor corresponding to the average displacements and ε^*_{ij} is fluctuating strain tensor corresponding to the oscillating displacements. As shown earlier, the fluctuating strain tensor is assumed to vary periodically. Now for the virtual displacement or weak form of the equilibrium equations let us assume that the virtual displacement (v) and hence the virtual strain $\varepsilon_{ij}(\mathrm{v})$ can also be expressed as asymptotic functions of x_i and y_i . Thus, the virtual strain is given as

$$\varepsilon_{ij}(\mathrm{V}) = \frac{1}{2}\left(\frac{\partial v_i^\eta}{\partial x_j} + \frac{\partial v_j^\eta}{\partial x_i}\right) = \frac{1}{2}\left[\left(\frac{\partial v_{0i}}{\partial x_j} + \frac{\partial v_{0j}}{\partial x_i}\right) + \left(\frac{\partial v_{1i}}{\partial y_j} + \frac{\partial v_{1j}}{\partial y_i}\right) + \eta\left(\frac{\partial v_{1i}}{\partial x_j} + \frac{\partial v_{1j}}{\partial x_i}\right)\right] + h.o.t. \quad (7.133)$$

Further, this strain can be written as average and microscopic strain due to virtual displacement as

$$\varepsilon_{ij}(\mathrm{v}) = \varepsilon^{(0)}_{ij}(\mathrm{v}) + \varepsilon^{(1)}_{ij}(\mathrm{v}), \varepsilon^{(0)}_{ij}(\mathrm{v}) = \frac{1}{2}\left(\frac{\partial u_{0i}}{\partial x_j} + \frac{\partial u_{0j}}{\partial x_i}\right), \varepsilon^{(1)}_{ij}(\mathrm{v}) = \frac{1}{2}\left(\frac{\partial u_{1i}}{\partial y_j} + \frac{\partial u_{1j}}{\partial y_i}\right) \quad (7.134)$$

The weak form of the equilibrium equations is given by

$$\int_{\Omega^\eta} C_{ijkl}\ \varepsilon_{ij}(\mathrm{v})\varepsilon_{kl}(\mathrm{u})d\Omega^\eta = \int_\Gamma T_i v_i d\Gamma \quad (7.135)$$

Here, Ω^η denotes the total, that is, macroscopic plus microscopic domain of the composite. The tractions T_i and the boundary displacements, if any, are applied only on the macroscopic boundaries of the composite. The first of Equation (7.132) and the first of Equation (7.134) are used in above equation. The resulting expanded form of the above equation is then given as

$$\int_{\Omega^\eta} C_{ijkl}\left(\varepsilon^{(0)}_{ij}(\mathrm{v}) + \varepsilon^{(1)}_{ij}(\mathrm{v})\right)\left(\bar{\varepsilon}_{kl}(\mathrm{u}) + \varepsilon^*_{kl}(\mathrm{u})\right)d\Omega^\eta = \int_\Gamma T_i v_i d\Gamma \quad (7.136)$$

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It should be noted that the virtual displacement (v) is any arbitrary displacement. It can be chosen to vary on macroscopic or microscopic level. If we choose (v) to vary only on macroscopic level and be a constant on microscopic level then we get the macroscopic equilibrium equation as

$$\int_{\Omega^\eta} C_{ijkl}\,\varepsilon_{ij}^{(0)}(\mathrm{v})\left(\bar{\varepsilon}_{kl}(\mathrm{u})+\varepsilon_{kl}^{*}(\mathrm{u})\right)d\Omega^\eta=\int_{\Gamma} T_i\,v_i\,d\Gamma \qquad (7.137)$$

Here, $\varepsilon_{ij}^{(1)}(\mathrm{v})=0$ for the chosen variation of virtual displacement. However, if we choose (v) to vary only on microscopic level and be a constant on macroscopic level then we get the microscopic equilibrium equation as

$$\int_{\Omega^\eta} C_{ijkl}\,\varepsilon_{ij}^{(1)}(\mathrm{v})\left(\bar{\varepsilon}_{kl}(\mathrm{u})+\varepsilon_{kl}^{*}(u)\right)d\Omega^\eta=0 \qquad (7.138)$$

Here, $\varepsilon_{ij}^{(0)}(\mathrm{v})=0$ for the chosen variation of virtual displacement. Since ε_{kl}^{*} varies periodically, Equation (7.137) and Equation (7.138) may be simplified assuming η approaching zero in the limit as

$$\int_{\Omega}\frac{1}{|V_{RVE}|}\left[\int_{V_{RVE}} C_{ijkl}\,\varepsilon_{ij}^{(0)}(\mathrm{v})\left(\bar{\varepsilon}_{kl}(\mathrm{u})+\varepsilon_{kl}^{*}(u)\right)dV_{RVE}\right]d\Omega=\int_{\Gamma} T_i\,v_i\,d\Gamma \qquad (7.139)$$

and

$$\int_{\Omega}\frac{1}{|V_{RVE}|}\left[\int_{V_{RVE}} C_{ijkl}\,\varepsilon_{ij}^{(1)}(\mathrm{v})\left(\bar{\varepsilon}_{kl}(\mathrm{u})+\varepsilon_{kl}^{*}(\mathrm{u})\right)dV_{RVE}\right]d\Omega=0 \qquad (7.140)$$

Equation (7.140) to be true, the integration term over the RVE should be zero. This leads to the following condition:

$$\int_{V_{RVE}} C_{ijkl}\,\varepsilon_{ij}^{(1)}(\mathrm{v})\varepsilon_{kl}^{*}(\mathrm{u})\,dV_{RVE}=-\int_{V_{RVE}} C_{ijkl}\,\varepsilon_{ij}^{(1)}(\mathrm{v})\bar{\varepsilon}_{kl}(\mathrm{u})\,dV_{RVE} \qquad (7.141)$$

Here, in general, the strain $\bar{\varepsilon}_{ij}$ is not known. However, for a linear problem, any arbitrary $\bar{\varepsilon}_{ij}$ can be written as linear combination of unit strains as given in the following equation. The unit strains in the following equation are given for 3*D* case.

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$$\bar{\varepsilon}_{ij}^{11} = -\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \bar{\varepsilon}_{ij}^{22} = -\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \bar{\varepsilon}_{ij}^{33} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
$$\bar{\varepsilon}_{ij}^{12} = -\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \bar{\varepsilon}_{ij}^{13} = -\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \bar{\varepsilon}_{ij}^{23} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \qquad (7.142)$$
$$\bar{\varepsilon}_{ij}^{21} = -\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \bar{\varepsilon}_{ij}^{31} = -\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \quad \bar{\varepsilon}_{ij}^{32} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Due to symmetry considerations one needs to consider only the first six strains components in the linear combination. Substituting these unit strains in right hand side of Equation (7.141) we get the stress tensor

$$\sigma_{ij}^{*kl} = C_{ijmn}\bar{\varepsilon}_{mn}^{kl}$$

Now, putting this stress tensor in Equation (7.141) we solve the resulting auxilliary problem as

$$\int_{V_{RVE}} C_{ijpm}\,\varepsilon_{ij}^{(1)}(\mathrm{v})\varepsilon_{pm}^{*kl}(\mathrm{u})dV_{RVE} = -\int_{V_{RVE}} \varepsilon_{ij}^{(1)}(\mathrm{v})\sigma_{ij}^{*kl}\,dV_{RVE} \qquad (7.143)$$

The periodicity of the strain field ε_{ij}^{*kl} is obtained by constraining equal displacements on opposite sides of RVE. Once ε_{ij}^{*kl} is determined, the solution to Equation (7.141) is obtained by

$$\varepsilon_{ij}^{*} = M_{ijkl}\,\bar{\varepsilon}_{kl}, M_{ijkl} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) - \varepsilon_{ij}^{*kl} \qquad (7.144)$$

where δ_{ij} is Kronecker delta and M_{ijkl} is the local structure tensor. When the relationship between local RVE strain and the average strain is substituted into the macroscopic equilibrium equations, we get

$$\int_{\Omega} \frac{1}{|V_{RVE}|}\left[\int_{V_{RVE}} C_{ijkl}\,M_{klpm}\,dV_{RVE}\right]\varepsilon_{ij}^{(0)}(\mathrm{v})\bar{\varepsilon}_{pm}(\mathrm{u})d\Omega = \int_{\Gamma} T_i\,v_i d\Gamma \qquad (7.145)$$

Here, it should be noted that the terms $\varepsilon_{ij}^{(0)}$ and $\bar{\varepsilon}_{pm}$ are outside the integration over the RVE as they represent the average strain, which is constant, over RVE. The homogenization approach gives the equivalent properties of the composite laminate. The effective stiffness tensor, $\bar{C}_{ijkl}$ is defined (as in standard mechanics approach in Equation (7.98))

$$\bar{C}_{ijkl} = \frac{1}{|V_{RVE}|}\int_{V_{RVE}} C_{ijpm}\,M_{pmkl}\,dV_{RVE} \qquad (7.146)$$

Using this effective stiffness tensor, the final form of macroscopic equilibrium equation may be written

as

$$\int_{\Omega} \bar{C}_{ijkl}\ \varepsilon_{ij}^{(0)}(\mathrm{v})\ \bar{\varepsilon}_{kl}(\mathrm{u})d\Omega = \int_{\Gamma} T_i\ v_i d\Gamma \qquad (7.147)$$

It is important to note that the effective stiffness tensor obtained from Equation (7.146) is independent of size of RVE due to periodicity assumption used in obtaining M_{ijkl} .

Note: The effective stiffness tensor obtained using homogenization approach is independent of size of RVE as periodicity assumption has been imposed on RVE. In case of standard mechanics such boundary conditions are not imposed. Hence, the effective stiffness obtained is dependent on the size of RVE. This fact can be explained by St. Venant's principle for applied displacement or traction boundary conditions. However, when St. Venant effect is not significant (as in case of analysis with multi cell RVE) the two approaches may yield the same results.

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Home Work:

1. What are the lacunas in standard mechanics approach?
2. Explain the importance of applied boundary conditions on RVE in determining the effective properties.
3. Explain in detail the concept of homogenization.
4. Show that for the one dimensional case as shown in Figure 7.9 the effective Young's modulus determined using homogenization approach is same as given by the standard mechanics approach.

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