y_1 axis to remove the rigid rotations around y_3 and y_2, respectively, and constraining the third DOF of a different node along y_2 axis to remove rigid rotation around y_1.

4. Solve the boundary value problem.

5. Compute the average of the strain field within the RVE and the six components of the average strain are the first column of the effective compliance matrix.

To compute the complete effective compliance matrix, we have to let one of the stress components to be 1 and all other components to be zero in turn. A total of six such numerical analyses are needed.

The *periodic boundary conditions* (PBCs) are given in terms of

$$t_i^+ = -t_i^- \qquad \chi_i^+ = \chi_i^- \tag{5.104}$$

where

$$\chi_i = u_i - y_j \varepsilon_{ij}^0 \tag{5.105}$$

denoting the displacement fluctuation functions and superscripts $+$ and $-$ denote the quantities on the corresponding periodic boundaries. Basically PBCs require that the tractions on the corresponding periodic boundaries equal and opposite in directions, and displacement fluctuation functions equal to each other on the corresponding periodic boundaries. It can be shown as follows that PBCs will vanish the surface integral in Eq. (5.11)

$$\frac{1}{V}\oint_{\partial V} n_k\left(\sigma_{ik} - \bar{\sigma}_{ik}\right)\left(u_i - y_j\bar{\varepsilon}_{ij}\right)dS = \frac{1}{V}\oint_{\partial V}\left(t_i - \bar{\sigma}_{ik}n_k\right)\chi_i dS \tag{5.106}$$

due to the fact that the tractions are opposite to each other and the fluctuation functions are equal to each other as required in Eq. (5.104). Thus PBCs satisfy the Hill-Mandel macrohomogeneity condition. It can also be shown that the average strain field within the RVE will be equal to ε_{ij}^0 as follows:

$$\begin{aligned}\bar{\varepsilon}_{ij} = \langle \varepsilon_{ij} \rangle = \left\langle \frac{1}{2}(u_{i,j} + u_{j,i}) \right\rangle = \left\langle \frac{1}{2}(\varepsilon_{ij}^0 + \varepsilon_{ji}^0 + \chi_{i,j} + \chi_{j,i}) \right\rangle \\ = \varepsilon_{ij}^0 + \frac{1}{2V}\oint_{\partial V} \chi_i n_j + \chi_j n_i dS = \varepsilon_{ij}^0\end{aligned} \tag{5.107}$$

due to the periodicity of the displacement fluctuation functions.

It is proven that KUBCs and SUBCs lead to upper and lower estimates of the effective properties, respectively, compared to PBCs. Predictions using KUBCs and SUBCs converge to those of PBCs with increasing RVE sizes [33, 34, 35]. It is also theoretically justified and numerically confirmed that PBCs provide the most reasonable estimates among the class of possible boundary conditions satisfying the Hill-Mandel macrohomogeneity condition [36]. In other words, PBC is the best boundary conditions to use for the RVE analysis. As most FEA is displacement based, only the the displacement fluctuation functions are required to be periodic and the periodic traction boundary conditions are automatically satisfied for a fine enough mesh with converged stress results. PBCs were originally given in [33]. However, PBCs are not extensively used in the RVE analysis using commercial FEA software until the recent arrival of coupled equation constraints in these software packages which enables convenient application of these conditions.

In summary, substituting the constitutive relations in Eq. (5.8) along with the infinitesimal strain definition into Eq. (5.3), we can obtain the following displacement-based formulation for the RVE analysis

$$(C_{ijkl}u_{k,l})_{,j} = 0 \tag{5.108}$$

subject to boundary conditions

$$\left(u_i - y_j\varepsilon^0_{ij}\right)^+ = \left(u_i - y_j\varepsilon^0_{ij}\right)^- \tag{5.109}$$

PBCs in Eq. (5.109) can be written explicitly for the RVE shown in Figure 5.6. For example for the periodic boundary surfaces normal to y_1, we will have the following relations for u_1 on both surfaces

$$\left(u_1 - y_1\varepsilon^0_{11} - y_2\varepsilon^0_{12} - y_3\varepsilon^0_{13}\right)^+ = \left(u_1 - y_1\varepsilon^0_{11} - y_2\varepsilon^0_{12} - y_3\varepsilon^0_{13}\right)^- \tag{5.110}$$

which implies the following

$$u_1^+ - u_1^- = d\varepsilon^0_{11} + (y_2^+ - y_2^-)\varepsilon^0_{12} + (y_3^+ - y_3^-)\varepsilon^0_{13} \tag{5.111}$$

We need to create a periodic finite element mesh so that there are corresponding nodes on periodic surfaces. In other words, for a node on $y_1 = \frac{d}{2}$ surface with coordinate (y_2^+, y_3^+), there is a corresponding node on $y_1 = -\frac{d}{2}$ with the same coordinates so that $y_2^- = y_2^+, y_3^- = y_3^+$. Then the periodic constraints in Eq. (5.111) can be simplified to be

$$u_1^+ - u_1^- = d\varepsilon^0_{11} \tag{5.112}$$

Similarly, we can write all the other constraints. The constraints relating the surfaces at $y_1 = \frac{d}{2}$ and $y_1 = -\frac{d}{2}$ are

$$\begin{aligned}
u_1(\frac{d}{2}, y_2, y_3) - u_1(-\frac{d}{2}, y_2, y_3) &= d\varepsilon^0_{11}\\
u_2(\frac{d}{2}, y_2, y_3) - u_2(-\frac{d}{2}, y_2, y_3) &= d\varepsilon^0_{21}\\
u_3(\frac{d}{2}, y_2, y_3) - u_3(-\frac{d}{2}, y_2, y_3) &= d\varepsilon^0_{31}
\end{aligned}$$

The constraints relating the surfaces at $y_2 = \frac{l}{2}$ and $y_2 = -\frac{l}{2}$ are

$$\begin{aligned}
u_1(y_1, \frac{l}{2}, y_3) - u_1(y_1, -\frac{l}{2}, y_3) &= l\varepsilon^0_{12}\\
u_2(y_1, \frac{l}{2}, y_3) - u_2(y_1, -\frac{l}{2}, y_3) &= l\varepsilon^0_{22}\\
u_3(y_1, \frac{l}{2}, y_3) - u_3(y_1, -\frac{l}{2}, y_3) &= l\varepsilon^0_{32}
\end{aligned}$$

The constraints relating the surfaces at $y_3 = \frac{h}{2}$ and $y_3 = -\frac{h}{2}$ are

$$\begin{aligned}
u_1(y_1, y_2, \frac{h}{2}) - u_1(y_1, y_2, -\frac{h}{2}) &= h\varepsilon^0_{13}\\
u_2(y_1, y_2, \frac{h}{2}) - u_2(y_1, y_2, -\frac{h}{2}) &= h\varepsilon^0_{23}\\
u_3(y_1, y_2, \frac{h}{2}) - u_3(y_1, y_2, -\frac{h}{2}) &= h\varepsilon^0_{33}
\end{aligned}$$

To carry out an RVE analysis using PBCs, one normally follows the following steps after creating a periodic finite element mesh.

1. Set one component in ε_{ij}^0 to be 1 and all the other components to be zero. Say for example $\varepsilon_{11}^0 = 1$ and $\varepsilon_{22}^0 = \varepsilon_{33}^0 = 2\varepsilon_{12}^0 = 2\varepsilon_{13}^0 = 2\varepsilon_{23}^0 = 0$.

2. Apply PBCs to the RVE according to Eq. (5.109). One can refer to the explicit expressions above for the corresponding nonzero strain component.

3. One also needs to remove the three translational rigid body motion by constraining three DOFs of an arbitrary node.

4. Solve the boundary value problem.

5. Compute the average of the stress field within the RVE and the six components of the average stress are the first column of the effective stiffness matrix.

To compute the complete effective stiffness matrix, we have to let one of the strain components to be 1 and all other components to be zero in turn. A total of six such numerical analyses are needed.

The effective properties computed by the RVE analysis can be used for the macroscopic analysis. After the macroscopic analysis, one can also perform a dehomogenization analysis to obtain the local strain and stress field for any material point of interest using the global strain $\bar{\varepsilon}_{ij}$ or $\bar{\sigma}_{ij}$ calculated by the macroscopic analysis. For both KUBCS and PBCs, we can provide the global strains as inputs for the dehomogenization analysis to compute the local strain and stress fields within the RVE. For SUBCs, we need to provide the global stresses as inputs for the dehomogenization analysis to compute the local strain and stress fields. It is noted that in the dehomogenization analysis, a complete global strain or stress state (all components are nonzero) can be applied to predict the local fields using the same type of boundary conditions by plugging the actual values of the global strain or stress fields into Eq. (5.102), (5.103), or (5.109).

5.8.2 Mathematical homogenization theory

Mathematical homogenization theory (MHT), also called asymptotic homogenization theory, despite its arcane mathematical derivation, is another popular micromechanics method. It is an application of the formal asymptotic method through a two-scale formulation [37, 16]. Its application in engineering has been popularized by its implementation using the finite element method [38, 18, 39, 19]. Although it was originally developed for periodic media formed by unit cells, it can be applied to RVEs because the material must be locally periodic for us to replace it with an effective homogenous material in the macroscopic structural analysis. For periodic media, the unit cell can be chosen as an RVE. In fact, it will be shown later that MHT is exactly the same as the RVE analysis with periodic boundary conditions. Thus, we will use the RVE only in later derivations with the understanding that the RVE is chosen to be a unit cell for a periodic material.

The two-scale formulation assumes that a field function of the original structure can be generally written as a function of the macro coordinates x_k and the micro coordinates y_j. Following [16], the partial derivative of a function $f(x_k, y_j)$ can be expressed as

$$\frac{\partial f(x_k, y_j)}{\partial x_i} = \frac{\partial f(x_k, y_j)}{\partial x_i}|_{y_j=\text{const}} + \frac{1}{\delta}\frac{\partial f(x_k, y_j)}{\partial y_i}|_{x_k=\text{const}} \equiv f_{|i} + \frac{1}{\delta} f_{,i} \qquad (5.113)$$