1 Periodic Homogenization

Considering a heterogeneous object Ω^ϵ with periodic microstructures of size ϵ, as shown schematically in Fig. 1, our goal is to find the homogenized elasticity tensor C^H as the effective elasticity tensor of the object (defined more rigorously below). Parameter ϵ determines the size of cell Y relative to the domain Ω^ϵ and permits us to perform asymptotic analysis.

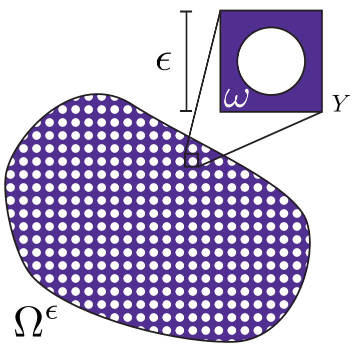

Figure 1 *(Schematic) Periodic tiling of a domain Ω with base cell Y having geometry ω and length scale ϵ.*

The elastic response of an object under external load $\mathbf{f}$ is governed by linear elasticity equation

$$-\nabla \cdot [C : \varepsilon(\mathbf{u}^\epsilon)] = \mathbf{f} \text{ in } \Omega^\epsilon, \tag{1}$$

complemented by appropriate boundary conditions. Considering a sequence of problems indexed by ϵ and letting $\mathbf{u}$ denote the limit of $\mathbf{u}^\epsilon$ as $\epsilon \to 0$, the homogenized elasticity tensor C^H is defined as the tensor that satisfies

$$-\nabla \cdot [C^H : \varepsilon(\mathbf{u})] = \mathbf{f} \text{ in } \Omega, \tag{2}$$

with same boundary conditions. Vectors $\mathbf{u}$ and $\mathbf{u}^\epsilon$ denotes the displacement, C is the local elasticity tensor, and $\varepsilon(\mathbf{u}) \coloneqq \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$ is the Cauchy strain tensor (defined similarly for $\mathbf{u}^\epsilon$).

Here we outline the periodic homogenization method using the two-scale asymptotic expansion method with minimal mathematical justification and refer the reader to [1, 2, 3] for more detail and rigorous justification. The mathematical difficulty of a framework that takes Eq. (1) to Eq. (2) is to define the proper notion of convergence as $\epsilon \to 0$. The two-scale method is based on the ansatz that for small ϵ, the family of solutions $\mathbf{u}^\epsilon$, parameterized by ϵ, can be written as

$$\mathbf{u}^\epsilon(\mathbf{x}) = \sum_{p=0}^{\infty} \epsilon^p \mathbf{u}_p\left(\mathbf{x}, \frac{\mathbf{x}}{\epsilon}\right). \tag{3}$$

Each term $\mathbf{u}_p(\mathbf{x}, \mathbf{y})$ is a Y-periodic function of $\mathbf{y}$.

The method of two-scale asymptotic expansions is a heuristic method and the above assumption is usually not correct after the first two terms; nonetheless, it is possible to rigorously justify the homogenization process and the convergence of the sequence $\mathbf{u}^\epsilon$ to the solution $\mathbf{u}$ (usually by means of the so-called energy method) [1, 2].

As implied by Eq. (2) and Eq. (3), the first term of the series $\mathbf{u}_0$ is identified with the solution of the homogenized equation $\mathbf{u}$. Knowing $\mathbf{u}$ for proper choices of $\mathbf{f}$, the effective elasticity tensor C^H can be computed. Note that the homogenized tensor C^H is almost never a spatial average of C.

To facilitate the analysis, let $\mathbf{x}$ denote the macroscopic variable and define $\mathbf{y} \coloneqq \mathbf{x}/\epsilon$ as the microscopic variable. For $\mathbf{y} \in Y$, the local elasticity tensor is given as

$$C(\mathbf{y}) = \begin{cases} C^{\text{base}} & \text{if } \mathbf{y} \in \omega, \\ 0 & \text{otherwise}, \end{cases} \tag{4}$$

where C^{base} is the known material property and is extended throughout Ω by Y-periodicity.

Let $\mathbf{e}^{kl} \coloneqq \frac{1}{2}(\mathbf{e}_k \otimes \mathbf{e}_l + \mathbf{e}_l \otimes \mathbf{e}_k)$ denote the canonical basis for symmetric rank 2 tensors and define $\mathbf{w}^{kl}$ as the microscopic displacements response for $\mathbf{e}^{kl}$ satisfying

$$\nabla \cdot (C^{\text{base}} : \varepsilon(\mathbf{w}^{kl})) = 0 \text{ in } \omega, \tag{5a}$$

$$[C^{\text{base}} : \varepsilon(\mathbf{w}^{kl})]\hat{\mathbf{n}} = -[C^{\text{base}} : \mathbf{e}^{kl}]\hat{\mathbf{n}} \text{ on } \partial\omega \backslash \partial Y, \tag{5b}$$

$$\mathbf{w}^{kl}(\mathbf{y}) \; Y\text{-periodic}, \tag{5c}$$

$$\int_\omega \mathbf{w}^{kl}(\mathbf{y})\, \mathrm{d}\mathbf{y} = \mathbf{0}, \tag{5d}$$

where the last constraint is to pin down the translational degrees of freedom; since we only care about strain $\varepsilon(\mathbf{w}^{kl})$. We refer to Eq. Set (5) as the cell problem.

Knowing $\mathbf{w}^{kl}$, the effective elasticity tensor is expressed as an integral over the cell Y

$$C^H_{ijkl} = \frac{1}{|Y|} \int_\omega C^{\text{base}}_{ijpq} [\varepsilon(\mathbf{w}^{kl})]_{pq} + C^{\text{base}}_{ijkl}\, \mathrm{d}\mathbf{y}. \tag{6}$$

See Appendix A for the connection between Eq. Set (5) and Eq. (6) and more detail on their derivation.

It is worth noting that C^H does not depend on the choice of domain Ω, force term $\mathbf{f}$, or boundary condition on $\partial\Omega$.

For each cell shape, Eq. Set (5) needs to be solved numerically for the six—instead of nine because of the symmetry in canonical basis ($\mathbf{e}^{kl} = \mathbf{e}^{lk}$)—cell problems to compute $\mathbf{w}^{kl}$ $(k, l = 1, 2, 3)$, which are in turn used to evaluate Eq. (6).

1.1 FEM Implementation

The cell problems (Eq. Set (5)) are solved numerically by FEM discretization of a single base cell. The volume integral (Eq. (6)) is computed on the same grid.

Given the wire network of the microstructure, defining its topology **[TODO: internal ref]**, a volume mesh is generated following the STRUT algorithm given in [4] involving the following steps: (i) A polygon is created around both ends of each segment. (ii) For each vertex, the convex hull of the nearby polygons and the vertex is constructed and the polygons themselves are removed from the hull. (iii) For each edge, the convex hull of its two polygons is constructed, and again the two polygons are removed from the hull. The volume mesh is then used to generated the tetrahedron elements for the FEM computation.

The linear elasticity solver needs to support periodic boundary conditions, which requires the tet-based volume mesh to have identical tessellation on opposite periodic cell faces. Periodic boundary conditions are implemented by direct elimination of variables. Direct elimination is performed by assigning all mesh or grid nodes in each connected component of the identified vertex graph the same degrees of freedom. For example, the cell's corner nodes—if they exist—appear as the graph's only component of size 8 and all get the same x, y, and z displacement degrees of freedom. Edge nodes will appear in a component of size 4.

To simplify operations such as rank 4 tensor inversion and double contractions, we use a symmetric tensor flattening approach to turn rank 4 tensors into matrices and rank 2 tensors into vectors. We end up storing the elasticity tensor as a symmetric 6×6 matrix with 21 coefficients. **[TODO: give ref]**.

A Asymptotic Analysis for Periodic Homogenization

As outlined in Section 1, the homogenization process proceeds by considering the solution of Eq. (1), the displacement $\mathbf{u}^\epsilon$, as $\epsilon \to 0$. One approach in taking this limit is through two-scale asymptotic expansions [1]. Further detail can be found in [1, 2], here we outline major steps in the derivation of C^H.

A.1 Two-scale Analysis

As mentioned in Section 1, the two-scale method is based on the ansatz that for small ϵ, the family of solutions $\mathbf{u}^\epsilon$, parameterized by ϵ, can be written as

$$\mathbf{u}^\epsilon(\mathbf{x}) = \sum_{p=0}^{\infty} \epsilon^p \mathbf{u}_p \left(\mathbf{x}, \frac{\mathbf{x}}{\epsilon}\right). \tag{7}$$

Each function $\mathbf{u}_p$ separates its dependence on $\mathbf{x}$ (i.e. the smoothly varying, macroscopic part) from its dependence on $\mathbf{y} = \mathbf{x}/\epsilon$ (the microscopic fluctuations). Plugging the series into Eq. (1), collecting coefficients of ϵ^p terms, and identifying each coefficient of ϵ^p of as an individual equation, yields a cascade of equations for $\mathbf{u}_p$

$$\epsilon^{-2}: \ -\nabla_{\mathbf{y}} \cdot [C(\mathbf{y}) : \varepsilon_{\mathbf{y}}(\mathbf{u}_0)] = \mathbf{0} \tag{8}$$

$$\begin{aligned} \epsilon^{-1}: \ & -\nabla_{\mathbf{y}} \cdot [C(\mathbf{y}) : (\varepsilon_{\mathbf{y}}(\mathbf{u}_1) + \varepsilon_{\mathbf{x}}(\mathbf{u}_0))] - \\ & \nabla_{\mathbf{x}} \cdot [C(\mathbf{y}) : \varepsilon_{\mathbf{y}}(\mathbf{u}_0)] = \mathbf{0}, \end{aligned} \tag{9}$$

$$\begin{aligned} \epsilon^{0}: \ & -\nabla_{\mathbf{y}} \cdot [C(\mathbf{y}) : (\varepsilon_{\mathbf{y}}(\mathbf{u}_2) + \varepsilon_{\mathbf{x}}(\mathbf{u}_1))] - \\ & \nabla_{\mathbf{x}} \cdot [C(\mathbf{y}) : (\varepsilon_{\mathbf{y}}(\mathbf{u}_1) + \varepsilon_{\mathbf{x}}(\mathbf{u}_0))] = \mathbf{f}, \end{aligned} \tag{10}$$

where the subscripts $\mathbf{x}$ or $\mathbf{y}$ imply derivative with respect to that variable. Eq. (8) is satisfied by a function independent of $\mathbf{y}$, $\mathbf{u}_0(\mathbf{x}, \mathbf{y}) \equiv \mathbf{u}(\mathbf{x})$. Using this, Eq. (9) implies a linear relationship between $\varepsilon_{\mathbf{y}}(\mathbf{u}_1)$ and $\varepsilon_{\mathbf{x}}(\mathbf{u})$, which we can express with a rank 4 tensor F such that

$$\varepsilon_{\mathbf{y}}(\mathbf{u}_1) = F : \varepsilon_{\mathbf{x}}(\mathbf{u}), \tag{11}$$

mapping macroscopic strain to microscopic fluctuation strain.

The term for ϵ^0 uniquely defines $\mathbf{u}_2$ based on $\mathbf{u}$ and $\mathbf{u}_1$ if and only if the compatibility condition of the Fredholm alternative (zero average right hand side) is satisfied. Integrating the ϵ^0 term, using Divergence theorem and periodicity of $\mathbf{u}_1$ and $\mathbf{u}_2$ we have

$$-\nabla_{\mathbf{x}} \cdot \int_Y C(\mathbf{y}) : [\varepsilon_{\mathbf{y}}(\mathbf{u}_1) + \varepsilon_{\mathbf{x}}(\mathbf{u})] \, d\mathbf{y} = |Y| \mathbf{f}.$$

Using Eq. (11)

$$-\nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{|Y|} \int_Y C(\mathbf{y}) : F + C(\mathbf{y}) \, d\mathbf{y} \right) : \varepsilon_{\mathbf{x}}(\mathbf{u}) \right] = \mathbf{f}, \tag{12}$$

Comparing this with Eq. (2) implies

$$C^H = \frac{1}{|Y|} \int_Y C(\mathbf{y}) : F + C(\mathbf{y}) \, d\mathbf{y} \tag{13}$$

A.2 Local Microscopic Displacement

It remains to determine rank 4 tensor F appearing in C^H using Eq. (9). Letting $\mathbf{e}^{kl}$ to denote canonical basis for symmetric rank 2 tensors:

$$\mathbf{e}^{kl} = \frac{1}{2}\left(\mathbf{e}_k \otimes \mathbf{e}_l + \mathbf{e}_l \otimes \mathbf{e}_k\right)$$

where $\mathbf{e}_k$ is the k^{th} canonical basis element. Then the macroscopic strain can be decomposed as $\varepsilon_{\mathbf{x}}(\mathbf{u}) = [\varepsilon_{\mathbf{x}}(\mathbf{u})]_{kl}\mathbf{e}^{kl}$. If Y-periodic $\mathbf{w}^{kl}(\mathbf{y})$ solves (9) for $\mathbf{e}^{kl}$:

$$-\nabla_{\mathbf{y}} \cdot (C(\mathbf{y}) : [\varepsilon_{\mathbf{y}}(\mathbf{w}^{kl}) + \mathbf{e}^{kl}]) = \mathbf{0}. \tag{14}$$

By linearity, $\varepsilon_{\mathbf{y}}(\mathbf{u}_1) = [\varepsilon_{\mathbf{x}}(\mathbf{u})]_{kl}\varepsilon_{\mathbf{y}}(\mathbf{w}^{kl})$, implying

$$F_{pqkl} = [\varepsilon_{\mathbf{y}}(\mathbf{w}^{kl})]_{pq} \tag{15}$$

Plugging this into the equation for the homogenized elasticity coefficients, we get

$$C^H_{ijkl} = \frac{1}{|Y|}\int_Y C_{ijpq}(\mathbf{y})[\varepsilon_{\mathbf{y}}(\mathbf{w}^{kl})]_{pq} + C_{ijkl}(\mathbf{y})\,\mathrm{d}\mathbf{y}. \tag{16}$$

Once we know each $\mathbf{w}^{kl}$, we can compute the homogenized elasticity tensor with a simple integration over the base cell. We find these by solving the 6 cell problems

$$-\nabla_{\mathbf{y}} \cdot (C(\mathbf{y}) : [\varepsilon_{\mathbf{y}}(\mathbf{w}^{kl}) + \mathbf{e}^{kl}]) = \mathbf{0} \quad \text{in } Y, \tag{17a}$$

$$\mathbf{w}^{kl}(\mathbf{y}) \ Y\text{-periodic}, \tag{17b}$$

$$\int_\omega \mathbf{w}^{kl}(\mathbf{y})\,\mathrm{d}\mathbf{y} = \mathbf{0}. \tag{17c}$$

One for each canonical basis tensor $\mathbf{e}^{kl}$. The last constraint is to fix the remaining transnational degree of freedom; since we only care about strain $\varepsilon_{\mathbf{y}}(\mathbf{w}^{kl})$, we can arbitrarily choose to enforce $\mathbf{0}$ average displacement over the microstructure geometry.

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