1 Periodic Homogenization

Considering a heterogeneous object Ω^ϵ with periodic heterogeneities of size ϵ, as shown schematically in Fig. 1, our goal is to find the homogenized elasticity tensor C^H_{ijkl} as the effective elasticity tensor of the microstructure. Parameter ϵ determines the size of cell Y relative to the domain Ω^ϵ and permits us to perform asymptotic analysis as ϵ goes to zero (Appendix A).

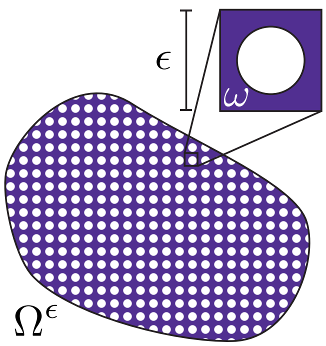

Figure 1 *(Schematic) Periodic tiling of a domain Ω with base cell Y having geometry ω and length scale ϵ.*

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

$$C_{ijkl}(\mathbf{y}) = \begin{cases} C^{\text{base}}_{ijkl} & \text{if } \mathbf{y} \in \omega, \\ 0 & \text{otherwise,} \end{cases} \tag{1}$$

where C^{base} is the known material property. We extend this function throughout Ω by Y-periodicity. The effective elasticity tensor is derived using two-scale asymptotic analysis on the material's elastic response and is expressed as an integral over the cell Y

$$C^H_{ijkl} = \frac{1}{|Y|} \int_\omega C^{\text{base}}_{ijpq}[\varepsilon(\mathbf{w}^{kl})]_{pq} + C^{\text{base}}_{ijkl} \, \mathrm{d}\mathbf{y}, \tag{2}$$

where $\varepsilon(\mathbf{w}) = \frac{1}{2}(\nabla \mathbf{w} + (\nabla \mathbf{w})^T)$ is the Cauchy strain tensor and $\mathbf{w}^{kl}$ are the microscopic displacements satisfying

$$\nabla \cdot (C^{\text{base}}_{ijmn}[\varepsilon(\mathbf{w}^{kl})]_{mn}) = 0 \quad \text{in } \omega, \tag{3a}$$

$$C^{\text{base}}_{ijmn}[\varepsilon(\mathbf{w}^{kl})]_{mn}\hat{n}_j = -C^{\text{base}}_{ijmn}[\mathbf{e}^{kl}]_{mn}\hat{n}_j \quad \text{on } \partial\omega \setminus \partial Y, \tag{3b}$$

$$\mathbf{w}^{kl}(\mathbf{y}) \ Y\text{-periodic}, \tag{3c}$$

$$\int_\omega \mathbf{w}^{kl}(\mathbf{y}) \, \mathrm{d}\mathbf{y} = \mathbf{0}, \tag{3d}$$

where $\mathbf{e}^{kl} \coloneqq \frac{1}{2}(\mathbf{e}_k \otimes \mathbf{e}_l + \mathbf{e}_l \otimes \mathbf{e}_k)$ are the canonical basis for symmetric rank 2 tensors. See Appendix A for more detail on the derivation of Eq. (2) and Eq. Set (3).

For each cell shape, Eq. Set (3) needs to be solved numerically for the six[1] cell problems to compute $\mathbf{w}^{kl}$ $(k, l = 1, 2, 3)$, which are in turn used to evaluate Eq. (2).

1.1 FEM Implementation

The cell problems (Eq. Set (3)) are solved numerically by FEM discretization of a single base cell. The volume integral (Eq. (2)) is computed on the same grid.

Two FEM implementations are used: (i) a traditional volume mesh discretization using linear tetrahedron elements, and (ii) a novel "mesh free" method using a grid of trilinear cubes not conforming to the object's boundary. The mesh free method works directly on an object's level set description and is more suited for tasks such as shape or topology optimization where the object will change frequently and remeshing is intractable.

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. The mesh free method has matching grid on periodic faces by construction and only requires the geometry itself to be periodic. 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 graphs 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.

In both solvers, 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.

[1] instead of nine because of the symmetry in canonical basis $\mathbf{e}^{kl} = \mathbf{e}^{lk}$.

A Two-scale Analysis

The elastic response of the material under external load $\mathbf{f}$ with Neumann and Dirichlet boundary condition on respectively Γ_N and Γ_D is governed by linear elasticity equation

$$\begin{aligned} -\nabla \cdot [C : e(\mathbf{u})] &= \mathbf{f} \quad \text{in } \Omega \\ \hat{\mathbf{n}} \cdot [C : e(\mathbf{u})] &= \tau \quad \text{on } \Gamma_N \\ \mathbf{u} &= \mathbf{u}_D \quad \text{on } \Gamma_D, \end{aligned} \tag{4}$$

where $\mathbf{u}$ is the displacement vector and $e(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ is the strain tensor.

One homogenization approach is based on the method of two-scale asymptotic expansions [1], which is a heuristic derivation of the homogenized elasticity tensor, but once this tensor is found it can be rigorously justified. Further detail can be found in [1], here we outline major steps in derivation of C^H.

Assuming that the solution can be written as an asymptotic expansion

$$\mathbf{u}^\epsilon(\mathbf{x}) = \sum_{p=0}^{\infty} \epsilon^p \mathbf{u}_p(\mathbf{x}, \mathbf{y}),$$

with $\mathbf{u}_p(\mathbf{x}, \mathbf{y})$ constrained to be Y-periodic in $\mathbf{y}$. Each of these functions 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. (4) and collecting coefficients of ϵ^p terms we have

$$\epsilon^0: \quad -\nabla_{\mathbf{y}} \cdot [C(\mathbf{y}) : e_{\mathbf{y}}(\mathbf{u}_2)] - \nabla_{\mathbf{x}} \cdot [C(\mathbf{y}) : e_{\mathbf{y}}(\mathbf{u}_1)] - \nabla_{\mathbf{y}} \cdot [C(\mathbf{y}) : e_{\mathbf{x}}(\mathbf{u}_1)] - \nabla_{\mathbf{x}} \cdot [C(\mathbf{y}) : e_{\mathbf{x}}(\mathbf{u}_0)] = \mathbf{f}, \tag{5}$$

$$\epsilon^{-1}: \quad -\nabla_{\mathbf{y}} \cdot [C(\mathbf{y}) : e_{\mathbf{y}}(\mathbf{u}_1)] - \nabla_{\mathbf{x}} \cdot [C(\mathbf{y}) : e_{\mathbf{y}}(\mathbf{u}_0)] - \nabla_{\mathbf{y}} \cdot [C(\mathbf{y}) : e_{\mathbf{x}}(\mathbf{u}_0)] = \mathbf{0}, \tag{6}$$

$$\epsilon^{-2}: \quad -\nabla_{\mathbf{y}} \cdot [C(\mathbf{y}) : e_{\mathbf{y}}(\mathbf{u}_0)] = \mathbf{0}, \tag{7}$$

where $e_{\mathbf{x}}(\mathbf{u}) := \frac{1}{2}\left(\nabla_{\mathbf{x}} \mathbf{u} + (\nabla_{\mathbf{x}} \mathbf{u})^T\right)$ is the macroscopic strain operator and $e_{\mathbf{y}}$ is the microscopic strain operator, defined similarly.

Eq. (7) implies that $\mathbf{u}_0(\mathbf{x}, \mathbf{y}) = \mathbf{u}(\mathbf{x})$, which by the Fredholm alternative is unique [1, Lemma 2.3.21].[2] Plugging in $\mathbf{u}(\mathbf{x})$ for $\mathbf{u}_0$ simplifies (6) to

$$-\nabla_{\mathbf{y}} \cdot (C(\mathbf{y}) : [e_{\mathbf{y}}(\mathbf{u}_1) + e_{\mathbf{x}}(\mathbf{u})]) = \mathbf{0}, \tag{8}$$

which uniquely defines $\mathbf{u}_1(\mathbf{x}, \mathbf{y})$ at each point $\mathbf{x}$ up to a constant once $\mathbf{u}$ is known. We can express this relationship with a rank 4 tensor F such that $e_{\mathbf{y}}(\mathbf{u}_1) = F : e_x((u))$ mapping macroscopic strain to microscopic fluctuation strain. Eq. (5) 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 Eq. (5), using Divergence theorem and periodicity of $\mathbf{u}_1$ and $\mathbf{u}_2$, we have the homogenized force balance equation

$$C^H := \frac{1}{|Y|} \int_Y C(\mathbf{y}) : F + C(\mathbf{y}) \, \mathrm{d}\mathbf{y} \tag{9}$$

$$C^H_{ijkl} = \frac{1}{|Y|} \int_Y C_{ijpq}(\mathbf{y}) F_{pqkl} + C_{ijkl}(\mathbf{y}) \, \mathrm{d}\mathbf{y} \tag{10}$$

$$-\nabla_{\mathbf{x}} \cdot \left[C^H : e_{\mathbf{x}}(\mathbf{u})\right] = \mathbf{f} \quad \text{in } \Omega. \tag{11}$$

A.1 Cell Problems

All that remains is to use (8) to determine rank 4 tensor F appearing in C^H. First we introduce the canonical basis for symmetric rank 2 tensors:

$$e^{ij} = \frac{1}{2}\left(\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i\right)$$

where $\mathbf{e}_i$ is the i^{th} canonical basis element.Then we can trivially expand the macroscopic strain at any point in this basis:

$$e_{\mathbf{x}}(\mathbf{u}) = e^{ij}[e_{\mathbf{x}}(\mathbf{u})]_{ij}$$

We now take advantage of linearity to state that if Y-periodic $\mathbf{w}^{ij}(\mathbf{y})$ solves (8) for $e_{\mathbf{x}}(\mathbf{u}) = e^{ij}$:

$$-\nabla_{\mathbf{y}} \cdot (C(\mathbf{y}) : [e_{\mathbf{y}}(\mathbf{w}^{ij}) + e^{ij}]) = \mathbf{0}, \tag{12}$$

Since this solution is unique up to a constant wrt. $\mathbf{y}$, we know that

$$e_{\mathbf{y}}(\mathbf{u}_1) = e_{\mathbf{y}}(\mathbf{w}^{ij}[e_{\mathbf{x}}(\mathbf{u})]_{ij}) = e_{\mathbf{y}}(\mathbf{w}^{ij})[e_{\mathbf{x}}(\mathbf{u})]_{ij},$$

which gives us the linear map from $e_{\mathbf{x}}(\mathbf{u})$ to $e_{\mathbf{y}}(\mathbf{u}_1)$

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

Plugging this into the equation for the homogenized elasticity coefficients, we get in index notation:

$$C^H_{ijkl} = \frac{1}{|Y|} \int_Y C_{ijpq}(\mathbf{y})[e_{\mathbf{y}}(\mathbf{w}^{kl})]_{pq} + C_{ijkl}(\mathbf{y}) \, \mathrm{d}\mathbf{y}. \tag{13}$$

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

[2] Intuitively, Eq. (7) is a force balance for $\mathbf{u}_0$ in each instance of the periodic cell.

6 cell problems:

$$\begin{aligned}
-\nabla_{\mathbf{y}} \cdot \left(C(\mathbf{y}) : [e_{\mathbf{y}}(\mathbf{w}^{ij}) + e^{ij}]\right) = \mathbf{0} \quad \text{in } Y \\
\mathbf{w}^{ij}(\mathbf{y}) \; Y\text{-periodic} \\
\int_{\omega} \mathbf{w}^{ij}(\mathbf{y}) \, \mathrm{d}\mathbf{y} = \mathbf{0},
\end{aligned} \tag{14}$$

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

B Solving the Cell Problems

The homogenization task has now been reduced to solving 6 cell problems. Using Eq. (1), the traction free boundary condition on the interior boundaries $\partial\omega \setminus \partial Y$, and the fact that macroscopic stress $C^{\text{base}} : e^{ij}$ is constant throughout the base cell, we have

$$-\nabla \cdot \left(C^{\text{base}} : e(\mathbf{w}^{ij})]\right) = \mathbf{0} \quad \text{in } \omega \tag{15a}$$

$$\hat{\mathbf{n}} \cdot \left[C^{\text{base}} : e(\mathbf{w}^{ij})\right] = -\hat{\mathbf{n}} \cdot \left[C^{\text{base}} : e^{ij}\right] \quad \text{on } \partial\omega \setminus \partial Y \tag{15b}$$

$$\mathbf{w}^{ij}(\mathbf{y}) \; Y\text{-periodic} \tag{15c}$$

$$\int_{\omega} \mathbf{w}^{ij}(\mathbf{y}) \, \mathrm{d}\mathbf{y} = \mathbf{0}, \tag{15d}$$

References

[1] G. Allaire. *Shape Optimization by the Homogenization Method*. Number v. 146 in Applied Mathematical Sciences. Springer, 2002.