



# How to determine composite material properties using numerical homogenization



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## ABSTRACT

Numerical homogenization is an efficient way to determine effective macroscopic properties, such as the elasticity tensor, of a periodic composite material. In this paper an educational description of the method is provided based on a short, self-contained Matlab implementation. It is shown how the basic code, which computes the effective elasticity tensor of a two material composite, where one material could be void, is easily extended to include more materials. Furthermore, extensions to homogenization of conductivity, thermal expansion, and fluid permeability are described in detail. The unit cell of the periodic material can take the shape of a square, rectangle, or parallelogram, allowing for all kinds of 2D periodicities.

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## 1. Introduction

The microstructure of composite materials, where two or more materials are combined to achieve a material with attractive properties, can often be described by a unit cell, which is periodically repeated in one or more directions, as illustrated in Fig. 1.

Such periodic, or almost periodic, microstructures can be found in materials such as fiber composites and bone. Information about the microstructure can be obtained by e.g. a CT-scan. The technique described in the following can thereafter be applied to find the effective properties of the material. For human bone this has been done by e.g. Hollister [1], who has also been among the first to apply the technique for the design of metal and polymer implants [2,3].

Assuming length scales where the theory of elasticity can be applied and perfect bonding between the different materials in the unit cell, homogenization can be used to compute the macroscopic composite material properties. Homogenization relies on an asymptotic expansion of the governing equations, which allows for a separation of scales. This is valid when there is a clear separation between the macro- and microscopic length scales. The theory behind homogenization is covered in detail in several works, some of the first being [4,5]. Another good theoretical introduction to the subject can be found in [6].

According to the theory of homogenization, the macroscopic elasticity tensor  $E_{ijkl}^H$  of a periodic composite material can be computed as:

$$E_{ijkl}^H = \frac{1}{|V|} \int_V E_{pqrs} (\varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^{(ij)}) (\varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^{(kl)}) dV \quad (1)$$

where  $|V|$  denotes the volume of the unit cell,  $E_{pqrs}$  is the locally varying stiffness tensor,  $\varepsilon_{pq}^{0(ij)}$  are prescribed macroscopic strain fields (in 2D there are three; e.g. unit strain in the horizontal direction (11), unit strain in the vertical direction (22), and unit shear strain (12 or 21)), while the locally varying strain fields  $\varepsilon_{pq}^{(ij)}$  are defined as:

$$\varepsilon_{pq}^{(ij)} = \varepsilon_{pq}(\chi^{ij}) = \frac{1}{2} (\chi_{p,q}^{ij} + \chi_{q,p}^{ij}) \quad (2)$$

based on the displacement fields  $\chi^{kl}$  found by solving the elasticity equations with a prescribed macroscopic strain

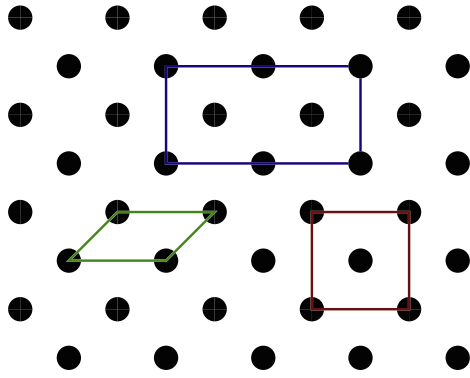
$$\int_V E_{ijpq} \varepsilon_{ij}(v) \varepsilon_{pq}(\chi^{kl}) dV = \int_V E_{ijpq} \varepsilon_{ij}(v) \varepsilon_{pq}^{0(kl)} dV \quad \forall v \in V \quad (3)$$

where  $v$  is a virtual displacement field. For most practical problems the homogenization is performed numerically by discretizing and solving Eq. (3) using e.g. the finite element method. This is often referred to as numerical homogenization. The numerical homogenization procedure is also well described in the literature. One of the first detailed descriptions of the procedure can be found in [7], while [8–10] provide a three paper review of both numerical homogenization and how it is used in conjunction with topology optimization to design periodic materials.

However, the implementation can still seem daunting, and with the small and self-contained Matlab example provided in Appendix A, we try to lower the barrier for using numerical homogenization. The code computes the homogenized elasticity tensor for a two

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**Fig. 1.** A section of a 2D periodic microstructure consisting of two materials (white and black). The red line encloses a square unit cell, the blue a rectangular unit cell, and the green a parallelogram unit cell. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

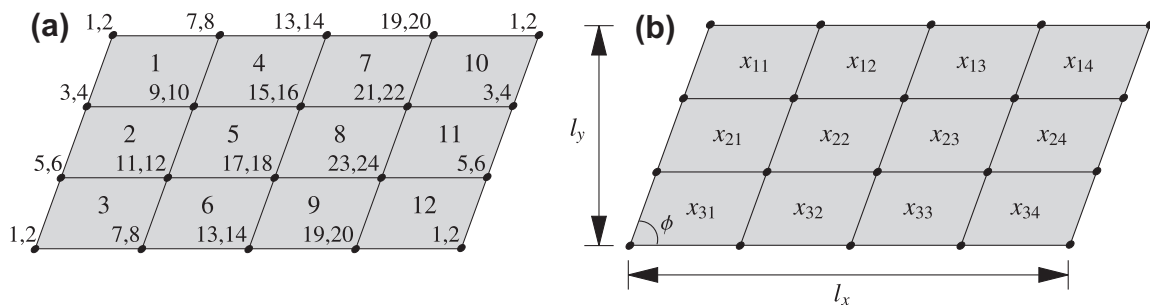
material composite. A detailed description of the implementation is provided in Section 2, while examples of extensions to three material composites, homogenized thermal expansion, and thermal conductivity are given in Section 3. Section 4 is devoted to a slightly more involved extension of homogenized permeability.

## 2. Matlab implementation

In the basic Matlab implementation we treat the case of a composite consisting of two materials. The unit cell is discretized using bilinear finite elements (plane strain elements are used, but plane stress can be specified by providing modified material data), and an indicator matrix  $x$  specifies whether a finite element contains material 1 ( $x_e = 1$ ) or material 2 ( $x_e = 2$ ).

In Fig. 2 the structure of the mesh used to discretize the unit cell and the indicator matrix  $x$  are illustrated. Fig. 2b also shows how the geometry of the unit cell is specified in the Matlab code. The homogenization function needs six user specified inputs. The two first arguments ( $l_x$  and  $l_y$ ) are the width,  $l_x$  and height,  $l_y$ , of the unit cell. The third argument ( $l_{\text{lambda}}$ ) is a vector containing Lamé's first parameter for material 1 and for material 2. Similarly, the fourth argument ( $mu$ ) is a vector with Lamé's second parameter for the two materials. The fifth argument ( $\phi$ ) is the angle,  $\phi$ , between the horizontal axis and the left wall in the unit cell. Finally, the sixth argument is the indicator matrix  $x$ . The discretization is determined from the size of  $x$ ; number of rows equals number of elements in the vertical direction, and number of columns equals number of elements in the horizontal direction.

Remark the angle  $\phi$  should be given in degrees and to avoid overly distorted elements it should not be smaller than  $45^\circ$  nor larger than  $135^\circ$ . As discussed in [11] a parallelogram unit cell allows for the analysis of general periodic materials, including polygonal cells.



**Fig. 2.** (a) Illustration of finite element mesh used to discretize unit cell (element numbers are big, and degrees of freedom are small) and (b) corresponding structure of indicator matrix  $x$ .

Calling the function in Appendix A as:

```
x = randi([1 2],200)
homogenize(1,1,[.01 2],[0.02 4],90,x)
```

will compute the effective properties of a random microstructure consisting of two materials, where the stiff material has an elasticity modulus of about 100 times the soft material. The homogenization is done by discretizing the unit cell with 200 times 200 bilinear elements, since that is the size of  $x$ . The different parts of the homogenization procedure implementation are explained in detail in the following.

If only a single material is used the stiffness will be constant throughout the unit cell resulting in zero displacements i.e.  $\varepsilon_{ij} = 0$  and the original stiffness is obtained when applying Eq. (1).

### 2.1. The element stiffness matrix and load vectors (lines 17 and 86–125)

The elasticity equation from (3) can be discretized using the finite element method. The left hand side, i.e. the stiffness matrix, yields:

$$\mathbf{K} = \sum_{e=1}^N \int_{V_e} \mathbf{B}_e^T \mathbf{C}_e \mathbf{B}_e dV_e \quad (4)$$

where the summation denotes the assembly of  $N$  finite elements. The matrix  $\mathbf{B}_e$  is the element strain–displacement matrix,  $V_e$  is the volume of element  $e$ , and  $\mathbf{C}_e$  is the constitutive matrix for the element, which for an isotropic material (we assume the materials used to build the composite are isotropic) is:

$$\mathbf{C}_e = \lambda_e \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \mu_e \cdot \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (5)$$

where  $\lambda_e$  and  $\mu_e$  are Lamé's first and second parameter for the material in element  $e$ , respectively. Lamé's parameters can be computed from Young's modulus  $E$  and the Poisson's ratio  $\nu$  using the relations:

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)} \quad (6)$$

And to get plane stress properties Lamé's first parameter must further be modified as follows:

$$\hat{\lambda} = \frac{2\mu\lambda}{\lambda + 2\mu} \quad (7)$$

In the initialization the element stiffness matrix is split into two corresponding parts, such that the stiffness matrix is a function of the material properties in the elements:

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