# 1 Analytic homogenization

## 1.1 Problem statement

Many physical problems are modelled by linear PDE (systems) of second order in a region $V$, the points of which are written as $\mathbf{x}$:

$$\mathrm{D}(\mathbf{x})[\mathbf{u}(\mathbf{x})] = \mathbf{g}(\mathbf{x}) \tag{1}$$

The location-dependent linear operator $\mathrm{D}(\mathbf{x})$ consists of taking the gradient, applying the constitutive linear mapping $C$, and taking the divergence:

$$\mathrm{D}(\mathbf{x})[\mathbf{u}(\mathbf{x})] = (C(\mathbf{x})[\mathbf{u}(\mathbf{x}) \otimes \nabla_{\mathbf{x}}]) \cdot \nabla_{\mathbf{x}} \tag{2}$$

The linear mapping $C[\cdot]$ is the constitutive law. It is an endomorphism that may have zero eigenvalues, as in case of linear elasticity, where the skew part of $\mathbf{u}(\mathbf{x}) \otimes \nabla_{\mathbf{x}}$ is mapped into $\mathbf{O}$. Throughout this pamphlet linear mappings are denoted by square brackets [], while parenthesis indicate a general dependence on the argument.

We can specify different physical problems in this framework. For example, for heat conduction we have

- $u(\mathbf{x})$: the scalar temperature field,
- $\nabla_{\mathbf{x}} u(\mathbf{x})$: the temperature gradient,
- $\mathbf{q}(\mathbf{x}) = -\mathbf{K}(\mathbf{x})[\nabla_{\mathbf{x}} u(\mathbf{x})]$: Fouriers law for heat conduction, with a positive definite symmetric second order heat conduction tensor $\mathbf{K}(\mathbf{x})$,
- $\nabla_{\mathbf{x}} \cdot \mathbf{q}(\mathbf{x}) = 0$: the stationary energy balance when only thermal energy is considered.

In case of elastostatics we have

- $\mathbf{u}(\mathbf{x})$: the vectorial displacement field,
- $\mathbf{u}(\mathbf{x}) \otimes \nabla_{\mathbf{x}}$: the displacement gradient $\mathbf{H}(\mathbf{x})$,
- $\mathbf{T}(\mathbf{x}) = \mathbb{C}(\mathbf{x}) \cdot \cdot \mathbf{H}(\mathbf{x})$: Hooke's law in three dimensions, with a positiv semidefinite stiffness tetrad $\mathbb{C}$,
- $\mathbf{T}(\mathbf{x}) \cdot \nabla_{\mathbf{x}} = \mathbf{o}$: the local balance of momentum without inertia and body forces.

Many problems, like diffusion and electrostatics fall into this scheme. On the boundary we have either Dirichlet or Neumann conditions, i.e. we prescribe $u_B(\mathbf{x})$ or $q_B = C[\nabla_{\mathbf{x}} u(\mathbf{x})]$, respectively.

Our concern is to find an average constitutive law $\overline{C}$ that replaces the reaction of the structured sample:

$$V[C(\mathbf{x})[\nabla_{\mathbf{x}} u(\mathbf{x})] = \overline{C} V[\nabla_{\mathbf{x}} u(\mathbf{x})] \tag{3}$$

The linear mapping $V[\cdot]$ is just the volume average. Usually, a different notation is employed, namely $\langle \cdot \rangle$. Since we will often exploit linearity, we stick to the linear function brackets $[\cdot]$. Please note that $\overline{C} \neq V[C(\mathbf{x})]$.

## 1.2 General solution

We can give a formal solution, which is in general hard to evaluate for specific cases

**Step 1.** We decompose $C(\mathbf{x})$ into a constant and a fluctuation part

$$C(\mathbf{x}) = C_0 + \tilde{C}(\mathbf{x}) \tag{4}$$

and replace it in the homogeneous PDE. We consider only the homogeneous PDE, since we want to determine the effective operator $\overline{C}$, which should not depend on specific right hand sides. This requirement renders the procedure useless for wave propagation problems. In that case, the differential operator $D$ takes a different form than presumed above. We consider the fluctuating part of the operator $D(\mathbf{x})$ as the right handside:

$$D_0 \mathbf{u}(\mathbf{x}) = -\tilde{D}(\mathbf{x}) \mathbf{u}(\mathbf{x}). \tag{5}$$

To the differential operator $D_0$ belongs an inverse operator, namely an integral with a Green function $G_0(\mathbf{x}, \mathbf{x}')$ that depends on the specific operator $D_0$. There will not appear another Green function, so we drop the index 0 on $G$. We use this to write the formal solution for Dirichlet- and Neumann problems

$$\mathbf{u}(\mathbf{x}) = -\int_V G(\mathbf{x}, \mathbf{x}')[\tilde{D}(\mathbf{x}')[\mathbf{u}(\mathbf{x}')]]\mathrm{d}\mathbf{x}' + \int_{\partial V} ....\mathrm{d}\mathbf{x}'. \tag{6}$$

Later, the boundary integrals are determined through the boundary conditions. Ultimately, these are not part of the solution, as we seek an effective material property. Therefore we disregard the details of these boundary integrals.

**Step 2.** We decompose $\tilde{D}$ into the derivatives and the linear mapping $\tilde{C}$, and extract the outer nabla operator by backward product. We do this in a purely symbolic manner here:

$$\int_V G(\mathbf{x}, \mathbf{x}')\{[\tilde{C}(\mathbf{x}')[\mathbf{u}(\mathbf{x}') \otimes \nabla_{\mathbf{x}'}]\} \cdot \nabla_{\mathbf{x}'}\mathrm{d}\mathbf{x}' = \tag{7}$$

$$\int_V \{G(\mathbf{x}, \mathbf{x}')[\tilde{C}(\mathbf{x}')[\mathbf{u}(\mathbf{x}') \otimes \nabla_{\mathbf{x}'}]\} \cdot \nabla_{\mathbf{x}'} - \{G(\mathbf{x}, \mathbf{x}')\} \otimes \nabla_{\mathbf{x}'}[\tilde{C}(\mathbf{x}')[\mathbf{u}(\mathbf{x}') \otimes \nabla_{\mathbf{x}'}]\mathrm{d}\mathbf{x}'. \tag{8}$$

The curly brackets indicate the term to which $\cdot\nabla_{\mathbf{x}'}$ is applied. Next, we convert the first volume integral into a boundary integral by Gauss's theorem an summarize it with the surface integrals that appeared before. The solution becomes

$$\mathbf{u}(\mathbf{x}) = -\int_V (G(\mathbf{x}, \mathbf{x}') \otimes \nabla_{\mathbf{x}'})[\tilde{C}(\mathbf{x}')[\mathbf{u}(\mathbf{x}') \otimes \nabla_{\mathbf{x}'}]\mathrm{d}\mathbf{x}' + \text{boundary integrals}. \tag{9}$$

**Step 3.** We apply the gradient $\nabla_{\mathbf{x}}$ to the solution. The nabla-operator is w.r.t. $\mathbf{x}$, thus we can pull it into the volume integral, where it only acts on the Green function. The gradient of the surface integrals would be needed if a specific boundary value problem is considered. We just summarize these to $\mathbf{H}_0$, being determined by the boundary conditions. For $\mathbf{u}(\mathbf{x}') \otimes \nabla_{\mathbf{x}'}$ we write $\mathbf{H}(\mathbf{x}')$.

$$\mathbf{H}(\mathbf{x}) = -\int_V (G(\mathbf{x}, \mathbf{x}') \otimes \nabla_{\mathbf{x}'} \otimes \nabla_{\mathbf{x}})[\tilde{C}(\mathbf{x}')[\mathbf{H}(\mathbf{x}')]]\mathrm{d}\mathbf{x}' + \mathbf{H}_0. \tag{10}$$

**Step 4.** We introduce the integral operator

$$\mathcal{G}[\mathbf{X}(\mathbf{x})] = \int_V (G(\mathbf{x}, \mathbf{x}') \otimes \nabla_{\mathbf{x}'} \otimes \nabla_{\mathbf{x}})[\mathbf{X}(\mathbf{x}')]\mathrm{d}x' \tag{11}$$

to shorten the expressions. Eq. (10) then becomes

$$\mathbf{H}(\mathbf{x}) = \mathbf{H}_0(\mathbf{x}) + \mathcal{G}[\tilde{C}(\mathbf{x}')[\mathbf{H}(\mathbf{x}')]]. \tag{12}$$

Next, we carry out an ensemble-averaging. This is indicated by $\langle\cdot\rangle$. It means that we consider many different realizations of the microstructure, all with the same boundary conditions, and all having the same statistical properties. This means, all realizations exhibit the same correlation functions. Further, we assume that ensemble-averaging of many smaller samples can be interchanged with volume-averaging of one very large sample. This property is called ergodicity. It does not hold for finite samples, as the boundary conditions are only vanishing for infinitely large samples. However, in our case the boundary conditions are eliminated, further, we can take the limit to $V \to \infty$ as Greens infinite body functions vanish then. The ensemble averaging results in

$$\langle\mathbf{H}\rangle = \mathbf{H}_0 + \mathcal{G}\langle\tilde{C}[\mathbf{H}]\rangle, \tag{13}$$

where we drop the dependence on $\mathbf{x}$ for convenience. Since the boundary conditions as well as the Green function are the same for all boundary value problems, and further the ensemble averaging is a linear operation, we can pull them out of the ensemble averaging (in case of $\mathcal{G}$) or drop the $\langle\cdot\rangle$ (in case of $\mathbf{H}_0$). We now solve the last equation for $\mathbf{H}_0$ and insert it backwards into the eq. (12) to eliminate the boundary conditions:

$$\mathbf{H}(\mathbf{x}) = \langle\mathbf{H}(\mathbf{x})\rangle + \mathcal{G}[\tilde{C}(\mathbf{x})[\mathbf{H}(\mathbf{x})] - \langle\tilde{C}(\mathbf{x})[\mathbf{H}(\mathbf{x})]\rangle] \tag{14}$$

The last equation is a Fredholm integral equation of the second kind. It is solved by successively applying the integral operation to $\langle \mathbf{H} \rangle$ and summing up these terms. We replace the linear integral operation by

$$\Gamma[\mathbf{X}] = \mathcal{G}[\tilde{C}[\mathbf{X}] - \langle \tilde{C}[\mathbf{X}] \rangle]. \tag{15}$$

With this abbreviation, the solution can be written as

$$\mathbf{H} = \sum_{n=0}^{\infty} \Gamma^n [\langle \mathbf{H} \rangle], \tag{16}$$

where we drop the dependence on $\mathbf{x}$.

**Step 5.** We put the formal result for $\mathbf{H}$ in the definition of $\overline{C}$. We replace the volume average with the ensemble average and use the decomposition of $C$, and pull out all homogeneous quantities of the averaging operations,

$$\overline{C}\langle \mathbf{H} \rangle = \langle C\mathbf{H} \rangle \tag{17}$$

$$= C_0\langle \mathbf{H} \rangle + \langle \tilde{C}\mathbf{H} \rangle \qquad = C_0\langle \mathbf{H} \rangle + \langle \tilde{C} \sum_{n=0}^{\infty} \Gamma^n \langle \mathbf{H} \rangle \rangle \tag{18}$$

$$= C_0\langle \mathbf{H} \rangle + \langle \tilde{C} \sum_{n=0}^{\infty} \Gamma^n \rangle \langle \mathbf{H} \rangle \tag{19}$$

Comparing coefficients gives us finally an expression for $\overline{C}$,

$$\overline{C} = C_0 + \langle \tilde{C} \sum_{n=0}^{\infty} \Gamma^n \rangle. \tag{20}$$

Carrying out the summation up to $n = 2$ we get

$$\overline{C} = C_0 + \langle \tilde{C} \rangle \qquad n = 0 \tag{21}$$

$$+ \langle \tilde{C}\mathcal{G}\tilde{C} \rangle - \langle \tilde{C} \rangle \mathcal{G} \langle \tilde{C} \rangle \qquad n = 1 \tag{22}$$

$$+ \langle \tilde{C}\mathcal{G}\tilde{C}\mathcal{G}\tilde{C} \rangle - \langle \tilde{C}\mathcal{G}\tilde{C} \rangle \mathcal{G} \langle \tilde{C} \rangle - \langle \tilde{C} \rangle \mathcal{G} \langle \tilde{C}\mathcal{G}\tilde{C} \rangle + \langle \tilde{C} \rangle \mathcal{G} \langle \tilde{C} \rangle \mathcal{G} \langle \tilde{C} \rangle \qquad n = 2 \tag{23}$$

One recognises that $\overline{C}$ is just the volume average in case of $n = 0$. In the higher order terms that contain multiple $\mathcal{G}$, the higher order correlation functions that capture the statistic properties of the microstructure are contained. This result can analogously be obtained for the inverse of $C$ (Dederichs and Zeller, 1973; Morawiec, 2004). The present deviation follows closely the proceeding of Morawiec (2004).

### 1.3 Important note

The choice $C_0$ has to be as general as possible to obtain the correct solution. For example, in case of istropic heat conduction in both phases, one might choose the identity tensor $\mathbf{I}$ for $\mathbf{C}_0$. Then, the anisotropy due to the distribution of the phases is not captured since $\tilde{C}$ and $G$ will be isotropic. Thus, one must presume $C_0$ to be the most general linear mapping in its space. This makes it very hard to determine the corresponding Green functions. At the same time, the higher order correlation functions are hard to obtain. In conclusion, a closed form solution can only be given for simple problems. On the other hand, one might determine the Green functions, the correlation functions and the integrals numerically.

## References


Dederichs, P.H. and R. Zeller (1973). "Variational treatment of the elastic constants of disordered materials". In: *Zeitschrift für Physik* 259, pp. 103–116.

Morawiec, A. (2004). *Orientations and Rotations– Computations in Crystallographic Textures*. Springer.