The Homogenization Method Applied to the Computation of Effective Thermal Conductivities of Composite Materials

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Summary

This is a thesis for the degree of Master of Science in Computer Engineering with Applied Mathematics specialization at Luleå University of Technology, Sweden. The thesis gives an insight to the subject of *Homogenization*. The homogenization theory has been developed in the studies of partial differential equations with rapidly oscillating coefficients. There are many important problems in for example mechanics and physics that can be modelled by partial differential equations of this type.

We use the homogenization method to compute effective thermal conductivities for composite material. A common feature for these materials is that the locally heterogeneous material behaves as a homogeneous medium, when the characteristic size of the inclusions is much smaller than the size of the whole sample. A direct numerical treatment of such problems are in general impossible due to the rapid variations on microscale level. Therefore one has to make some type of averaging. It turns out that the homogenization method is well suited to model and solve problems of this type.

We have developed a computer program that computes these effective conductivities. The program is mainly a finite element program, but it also has routines for the construction of unit cells, data loading/saving, computation of homogenized coefficients and graph plotting. The program supports both quadratic and hexagonal unit cells, and other types of unit cells can be constructed by the unit cell entering command. However, the main advantage with this program is that it supports periodic boundary conditions. Finally, the results of the computation are compared with various bounds. These bounds are very loose, so little information can be gained from them. With our program, one can restrict the intervals of the conductivities with orders of magnitude.

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Abstract

To solve boundary value problems of stationary heat distribution in composite materials, one has to solve partial differential equations with rapidly oscillating coefficients. These equations are in general impossible to solve numerically by standard methods. Instead, one wants to find constant, effective conductivities and solve the corresponding boundary value problem to get an approximate solution to the original problem. To compute these effective parameters, we have developed a finite element computer program with integrated homogenization routines.

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Chapter 1

Introduction

Because of the highly increased use of fibre reinforced composite materials, it is necessary to have mathematical methods for the prediction of material properties. The actual distribution of different phases of the composite is more or less unknown, but a reasonable assumption is that the structure of the material is periodic. This assumption leads to differential equations with periodically oscillating coefficients describing the spatial structure of the material. For instance, consider an elliptic boundary value problem modelling a stationary heat distribution in a region $\Omega \subset \mathbf{R}^n$ without internal heat source

$$-\frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial \tilde{u}}{\partial x_j}\right) = 0 \text{ in } \Omega,\ 1 \leq i,j \leq n \tag{1.1}$$

$$\tilde{u} = \tilde{u}_0 \text{ on } \partial\Omega, \tag{1.2}$$

where $a_{ij}(x)$, $\tilde{u}(x)$ and $\tilde{u}_0(x)$ denotes the thermal conductivity tensor, the temperature field and the boundary temperature. In the above formulation, we have used the Einstein summation convention for repeated indices, and if nothing else is indicated, we will use it in the sequel. This problem can be reformulated as

$$L(u) = -\frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right) = f(x) \text{ in } \Omega, \tag{1.3}$$

$$u = 0 \text{ on } \partial\Omega, \tag{1.4}$$

by finding a function $g(x)$ such that $g(x) = \tilde{u}_0(x)$ on $\partial\Omega$. Then $\tilde{u}(x) = u(x) + g(x)$ and $f(x) = \frac{\partial}{\partial x_i}(a_{ij}(x)\frac{\partial g}{\partial x_j})$. This problem is easily solved numerically

when the tensor $a_{ij}(x)$ is constant or slowly varying in x. But when $a_{ij}(x)$ oscillates rapidly in x, the numerical solution becomes cumbersome. This is because a very fine subdivision of the region is required to obtain an accurate solution. Instead, one wants to find an approximate solution of the problem by replacing $a_{ij}(x)$ by a constant conductivity tensor $q_{ij}(x)$ and solve the corresponding problem by some standard method. This constant tensor is called the *effective conductivity tensor* and may be found by an averaging procedure called the *homogenization method*.

The main idea of homogenization is the following: Let Ω be a domain with boundary $\partial\Omega$. For a fixed real number $\varepsilon > 0$, let A^ε be a linear partial differential operator on Ω and study the boundary value problem

$$A^\varepsilon u^\varepsilon = f^\varepsilon \tag{1.5}$$

in Ω.

It is here assumed that Ω is divided into identical cells of a size of order ε. By varying ε we obtain a family of partial differential operators $\{A^\varepsilon\}$ and a corresponding family of solutions $\{u^\varepsilon\}$. Then, a multiple scales expansion of the type $u^\varepsilon = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + ...$ is made.

If certain conditions are fulfilled (see e.g. Persson et al. [15]), then as $\varepsilon \to 0$, u^ε converges in a weak sense to u_0, where u_0 is the unique solution to the problem

$$A^0 u_0 = f \ , \tag{1.6}$$

where the coefficients of the homogenized operator A^0 are constant.

1.1 Notations and conventions

Let Ω denote an open and bounded set in $\mathbf{R}^n$ with boundary $\partial\Omega$. We say that Ω has the Lipschitz property if $\partial\Omega$ is locally Lipschitz, that is, if each point x of $\partial\Omega$ has a neighborhood U_x such that the intersection of U_x and $\partial\Omega$ is the graph of a Lipschitz continuous function. We define some vector spaces of real valued functions on Ω and their corresponding norms ($1 \leq p, q < \infty$):

$$C_0^\infty(\Omega) = \{u : u \text{ is smooth with support on a compact set } K \subset \Omega\},$$

$$L^p(\Omega) = \{u : \int_\Omega |u|^p \, dx < \infty\},$$

$$\|u\|_{L^p(\Omega)} = (\int_\Omega |u|^p \, dx)^{\frac{1}{p}},$$

$$L^\infty(\Omega) = \{u : \operatorname*{essup}_{x\in\Omega} |u(x)| < \infty\},$$

$$\|u\|_{L^\infty(\Omega)} = \operatorname*{essup}_{x\in\Omega} |u(x)|\,,$$

$$H^{1,p}(\Omega) = \{u \in L^p(\Omega) : \frac{\partial u}{\partial x_i} \in L^p(\Omega),\ i = 1, 2, ..., n\},$$

$$\|u\|_{H^{1,p}(\Omega)} = (\|u\|_{L^p(\Omega)}^p + \sum_{i=1}^n \left\| \frac{\partial u}{\partial x_i} \right\|_{L^p(\Omega)}^p)^{\frac{1}{p}},$$

$$H_0^{1,p}(\Omega) = \{u \in H^{1,p}(\Omega) : u = 0 \text{ on } \partial\Omega\},$$

$$\|u\|_{H_0^{1,p}(\Omega)} = \|u\|_{H^{1,p}(\Omega)}\,,$$

$$H^{1,p}(\Omega)/\mathbf{R} = \{u - c : u \in H^{1,p}(\Omega) \text{ and } c \in \mathbf{R}\},$$

$$\|u\|_{H^{1,p}(\Omega)/\mathbf{R}} = \inf_{c\in\mathbf{R}} \|u - c\|_{H^{1,p}(\Omega)}\,.$$

In $H^{1,p}(\Omega)$, the derivatives $\frac{\partial u}{\partial x_i}$ are taken in the distributional sense, that is, $\frac{\partial u}{\partial x_i}$ is the (unique) L^p-function that fulfills $\int_\Omega \frac{\partial u}{\partial x_i}\eta dx = -\int_\Omega u\frac{\partial \eta}{\partial x_i}dx$ for all test functions $\eta \in C_0^\infty(\Omega)$.

In $H_0^{1,p}(\Omega)$, $u = 0$ on Ω in the trace sense, that is, $\gamma u = 0$ where $\gamma : H^{1,p}(\Omega) \to L^p(\partial\Omega)$ is the unique bounded linear operator which fulfills $\gamma u = u|_{\partial\Omega}$ for all $u \in H^{1,p}(\Omega)$ that is continuous up to the boundary. The existence and uniqueness of the trace operator γ is a special case of the trace theorem, given in Alt [1], p. 190.

In the factor space $H^{1,p}(\Omega)/\mathbf{R}$ we identify functions u and v such that $u - v = c$, c constant.

For the case $p = 2$ we simply write $H^1(\Omega)$ and $H_0^1(\Omega)$ instead of $H^{1,2}(\Omega)$ and $H_0^{1,2}(\Omega)$, respectively.

By solutions of the boundary value problem (1.3) - (1.4) we understand weak solutions, that is solutions taken in the distributional sense. This means that we will consider functions $u \in H_0^1(\Omega)$ satisfying

$$a(u, v) = (f, v) \text{ for all } v \in H_0^1(\Omega), \tag{1.7}$$

where the bilinear form $a : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbf{R}$ is given by

$$a(u, v) = \int_\Omega a_{ij}(x) \frac{\partial u}{\partial x_j} \frac{\partial v}{\partial x_i} dx, \tag{1.8}$$

and the linear functional (f, v) by

$$(f, v) = \int_\Omega f v dx. \tag{1.9}$$

However, in the following chapters, we will consider an even more general boundary condition, leading to another definition of the linear functional. In (1.8) and (1.9), we have the restrictions $a_{ij}(x) \in L^\infty(\Omega)$ and $f \in L^2(\Omega)$. We will use $\langle \cdot \rangle$ to denote the arithmetic mean over a domain D, that is

$$\langle f \rangle = \frac{1}{m(D)} \int_D f dx, \tag{1.10}$$

where $m(D)$ is the Lebesgue measure (area in $\mathbf{R}^2$) of D. Later, D will be the Y-cell which we will define in the following chapter. We will write $|Y|$ instead of $m(Y)$.

Chapter 2

The Homogenization Method in $\mathbf{R}^2$

2.1 The model problem

Let Ω be a region in $\mathbf{R}^2$ with boundary $\partial\Omega$ containing two different isotropic materials, material 1 and material 2, each of them possessing a constant thermal conductivity. Assume that material 1 occupies the region $\Omega_1 \subset \Omega$ and that material 2 occupies the region $\Omega_2 = \Omega \setminus \Omega_1$. Furthermore, assume that the boundary $\partial\Omega$ can be divided into two disjunct parts, Γ_1 and Γ_2, that is $\partial\Omega = \Gamma_1 \cup \Gamma_2$ and $\Gamma_1 \cap \Gamma_2 = \emptyset$. Let $a_{ij}(x)$, $u(x)$, $f(x)$ and $g(x)$ denote the thermal conductivity tensor, the temperature field, the internal heat source density and the heat flow, respectively, at the spatial point x. Finally, let $n = (n_i)$ denote the outer unit normal to $\partial\Omega$. Then the temperature distribution in the material is given by the elliptic boundary value problem

$$-\frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right) = f(x) \text{ in } \Omega, \tag{2.1}$$

$$u = 0 \text{ on } \Gamma_1 \text{ and } a_{ij}(x)\frac{\partial u}{\partial x_j}n_i = g \text{ on } \Gamma_2. \tag{2.2}$$

The above equation is satisfied in each of the regions Ω_1 and Ω_2, together with the imposed boundary conditions. To get a well-posed problem in Ω, we assume the physically based conditions that the temperature and the normal components of the heat flows are continuous at the interfaces between Ω_1 and Ω_2. Let us from now on assume that material 2 is distributed in material 1.

For materials with few interfaces, we can easily solve the problem. But for geometries with several interfaces, the conductivity tensor $a_{ij}(x)$ is rapidly oscillating with x and the problem becomes hard to solve numerically. A special case of this is a fibre composite, where material 2 are fibres (for instance glass) distributed in a continuous matrix of material 1 (for instance epoxy).

The composite material is assumed to have a periodic structure, so that $\mathbf{R}^2$ can be divided into identical unit cells Y. Specifically, we will use quadratic or hexagonal unit cells in the numerical treatment of the problem. This assumption implies that the conductivity tensor $a_{ij}(x)$ must be periodic. To describe the Y-cell, we will use a local variable y defined as $y = x/\varepsilon$. Here, the parameter $\varepsilon > 0$ is a scale factor such that the conductivity tensor for the body is defined as $a^{\varepsilon}_{ij}(x) = a_{ij}(x/\varepsilon)$ for $x \in \Omega$.

The material is then described by a Y-periodic conductivity tensor $a_{ij}(y)$, defined on $\mathbf{R}^2$, where Y-periodicity means that $a_{ij}(y_1) = a_{ij}(y_2)$ whenever y_1 and y_2 have the same positions in the corresponding cells. In particular, we note that in a cell Y, Y-periodic functions take on the same boundary values twice, but with opposite outer normals $n = (n_i)$. Thus, for a Y-periodic vector field $(f_i(y))$,

$$\int_Y \frac{\partial f_i}{\partial y_i} dy = \oint_{\partial Y} f_i n_i ds = 0 \tag{2.3}$$

by Gauss' theorem. This is a crucial fact that will be frequently used in the sequel. Above, ds denotes the curve element of $\partial\Omega$. Further, we assume that $a_{ij}(y)$ belongs to $L^{\infty}(\Omega)$ and that $a_{ij}(y)$ is positive definite, that is

$$a_{ij}(y)\xi_i\xi_j \geq \alpha\xi_i\xi_i \tag{2.4}$$

for some $\alpha > 0$. Now we let ε vary and thereby obtain a class of boundary value problems

$$-\frac{\partial}{\partial x_i}\left(a^{\varepsilon}_{ij}(x)\frac{\partial u^{\varepsilon}}{\partial x_j}\right) = f^{\varepsilon}(x) \text{ in } \Omega, \tag{2.5}$$

$$u^{\varepsilon} = 0 \text{ on } \Gamma_1 \text{ and } a^{\varepsilon}_{ij}(x)\frac{\partial u^{\varepsilon}}{\partial x_j} n_i = g \text{ on } \Gamma_2. \tag{2.6}$$

2.2 Asymptotic expansion

To solve (2.5) with the boundary conditions (2.6), we will perform a multiple scales expansion (see e.g. Nayfeh [13]) of the solution u^{ε} in (2.5). We assume

that u^ε and f^ε can be represented by asymptotic expansions of the form

$$u^\varepsilon(x) = w_0(x,y) + \varepsilon w_1(x,y) + \varepsilon^2 w_2(x,y) + ...$$

$$f^\varepsilon(x) = f_0(x,y) + \varepsilon f_1(x,y) + \varepsilon^2 f_2(x,y) + ...$$

respectively, where w_i, $i = 0, 1, 2, ...$, are assumed to be Y-periodic in the variable y, where

$$y_i = \frac{x_i}{\varepsilon}. \tag{2.7}$$

We define the operators A^ε by

$$A^\varepsilon \Psi = -\frac{\partial}{\partial x_i}(a_{ij}^\varepsilon(x)\frac{\partial \Psi}{\partial x_j}). \tag{2.8}$$

By setting $\Psi(x) = \Phi(x,y)$ we get

$$\frac{\partial \Psi}{\partial x_i} = \frac{\partial \Phi}{\partial x_i} + \frac{1}{\varepsilon}\frac{\partial \Phi}{\partial y_i} \tag{2.9}$$

by the chain rule so that

$$A^\varepsilon \Psi = -\frac{\partial}{\partial x_i}(a_{ij}^\varepsilon(x)\frac{\partial \Psi}{\partial x_j}) = -(\frac{\partial}{\partial x_i} + \frac{1}{\varepsilon}\frac{\partial}{\partial y_i})(a_{ij}(y)(\frac{\partial \Phi}{\partial x_j} + \frac{1}{\varepsilon}\frac{\partial \Phi}{\partial y_j})) =$$

$$= -[a_{ij}(y)\frac{\partial^2 \Phi}{\partial x_i \partial x_j} + a_{ij}(y)\frac{1}{\varepsilon}\frac{\partial^2 \Phi}{\partial x_i \partial y_j} + \frac{1}{\varepsilon}\frac{\partial a_{ij}(y)}{\partial y_i}\frac{\partial \Phi}{\partial x_j} + \frac{1}{\varepsilon}a_{ij}(y)\frac{\partial^2 \Phi}{\partial y_i \partial x_j} +$$

$$+\frac{1}{\varepsilon^2}\frac{\partial a_{ij}(y)}{\partial y_i}\frac{\partial \Phi}{\partial y_j} + \frac{1}{\varepsilon^2}a_{ij}(y)\frac{\partial^2 \Phi}{\partial y_i \partial y_j}]. \tag{2.10}$$

We can therefore represent A^ε as

$$A^\varepsilon \Psi = (\varepsilon^{-2}A_0 + \varepsilon^{-1}A_1 + A_2)\Phi, \tag{2.11}$$

where

$$A_0 = -\frac{\partial}{\partial y_i}(a_{ij}(y)\frac{\partial}{\partial y_j}), \tag{2.12}$$

$$A_1 = -\frac{\partial}{\partial y_i}(a_{ij}(y)\frac{\partial}{\partial x_j}) - a_{ij}(y)\frac{\partial^2}{\partial x_i \partial y_j}, \tag{2.13}$$

$$A_2 = -a_{ij}(y)\frac{\partial^2}{\partial x_i \partial x_j}. \tag{2.14}$$

Equation (2.5) then becomes

$$A^\varepsilon u^\varepsilon(x) = (\varepsilon^{-2}A_0 + \varepsilon^{-1}A_1 + A_2)(w_0 + \varepsilon w_1 + \varepsilon^2 w_2 + ...) =$$
$$= \varepsilon^{-2}A_0 w_0 + \varepsilon^{-1}(A_0 w_1 + A_1 w_0) + (A_0 w_2 + A_1 w_1 + A_2 w_0) + ... =$$
$$= f_0 + \varepsilon f_1 + \varepsilon^2 f_2 + ... \tag{2.15}$$

Identification of powers of ε gives the three lowest order equations

$$A_0 w_0 = 0, \tag{2.16}$$

$$A_0 w_1 + A_1 w_0 = 0, \tag{2.17}$$

$$A_0 w_2 + A_1 w_1 + A_2 w_0 = f_0. \tag{2.18}$$

To solve (2.16) - (2.18), we need the following lemma:

Lemma 1 *Consider the boundary value problem*

$$A_0 \Phi = F \text{ in a unit } Y\text{-cell}, \tag{2.19}$$

where Φ is Y-periodic and $F \in L^2(Y)$. Then the following holds:

1. *There exists a weak Y-periodic solution Φ if and only if $\langle F \rangle = 0$.*
2. *If there exists a weak Y-periodic solution Φ, then it is unique up to an additive constant, that is, if we find one solution $\Phi_0(y)$, every solution is of the form $\Phi(y) = \Phi_0(y) + c$, where c is a constant.*

Proof: See Chapter 4, page 21.

The operator A_0 contains only derivatives with respect to y, so x is just a parameter in the solution of (2.16). We note that one solution to (2.16) is $w_0(x, y) \equiv 0$. Then, by Lemma 1, $w_0(x, y)$ is a solution of (2.16) if and only if w_0 is a constant with respect to the variable y, that is,

$$w_0(x, y) = u(x) \tag{2.20}$$

for some sufficiently differentiable function $u(x)$. By (2.17), (2.20) and (2.13), we get

$$A_0 w_1 = -A_1 w_0 = \frac{\partial a_{ij}}{\partial y_i}(y)\frac{\partial u}{\partial x_j}(x). \tag{2.21}$$

Here again, x is just a parameter because of the construction of A_0, so that the equation (2.21) may be regarded as a problem depending on the variable y only. Therefore it suffices to consider the *cell problem*

$$A_0\chi^k = -\frac{\partial a_{ik}}{\partial y_i}(y),\ \chi^k(y)\ Y\text{-periodic.} \tag{2.22}$$

Now, assume that a solution $\chi^k(y)$ of (2.22) is given. From Lemma 1 and the fact that A_0 does not include differentiation with respect to x, we can conclude that every solution to (2.22) is of the form

$$\chi_1^k(x,y) = \chi^k(y) + \tilde{u}_1^k(x), \tag{2.23}$$

since by (2.3) and the Y-periodicity of $a_{ij}(y)$

$$\left\langle \frac{\partial a_{ij}}{\partial y_i} \right\rangle = \frac{1}{|Y|}\int_Y \frac{\partial a_{ij}}{\partial y_i}dy = \frac{1}{|Y|}\oint_{\partial Y} a_{ij}n_i ds = 0. \tag{2.24}$$

By using linearity we get that

$$w_1(x,y) = -\chi^k(y)\frac{\partial u}{\partial x_k}(x) + u_1(x) \tag{2.25}$$

is a solution to (2.21), where $u_1(x) = -\tilde{u}_1^k(x)\frac{\partial u}{\partial x_k}(x)$, and, as pointed out above, every solution to (2.21) is of this form. Furthermore, by rewriting (2.18) as $A_0w_2 = f_0 - A_1w_1 - A_2w_0$ and using Lemma 1 once more, we conclude that (2.18) possesses a Y-periodic solution if and only if

$$\int_Y (f_0 - A_1w_1 - A_2w_0)dy = 0. \tag{2.26}$$

By inserting the expressions (2.20) and (2.25) for w_0 and w_1, respectively, into (2.26) we get

$$\int_Y (f_0 - \frac{\partial}{\partial y_i}(a_{ij}\chi^k)\frac{\partial^2 u}{\partial x_j \partial x_k} + \frac{\partial a_{ij}}{\partial y_i}\frac{\partial u_1}{\partial x_j} -$$

$$-a_{ij}\frac{\partial \chi^k}{\partial y_j}\frac{\partial^2 u}{\partial x_i \partial x_k} + a_{ij}\frac{\partial^2 u}{\partial x_i \partial x_j})dy = 0 \tag{2.27}$$

Since the functions $\chi^k(y)$ and $a_{ij}(y)$ are Y-periodic and the functions $u(x)$ and $u_1(x)$ are independent of y, the second and third term in (2.27) vanish by Gauss' theorem (2.3), and (2.27) is reduced to

$$\int_Y (f_0 - a_{ij}\frac{\partial \chi^k}{\partial y_j}\frac{\partial^2 u}{\partial x_i \partial x_k} + a_{ik}\frac{\partial^2 u}{\partial x_i \partial x_k})dy = 0, \tag{2.28}$$

which can be rewritten as

$$-\left[\int_y (a_{ik} - a_{ij}\frac{\partial \chi^k}{\partial y_j})dy\right]\frac{\partial^2 u}{\partial x_i \partial x_k} = \int_Y f_0(x)dy = \langle f_0 \rangle |Y| . \tag{2.29}$$

Dividing both sides with $|Y|$ gives

$$-q_{ik}\frac{\partial^2 u}{\partial x_i \partial x_k} = \langle f_0 \rangle , \tag{2.30}$$

which is the *homogenized equation*, where the *homogenized coefficients* q_{ik} are given by

$$q_{ik} = \left\langle a_{ik} - a_{ij}\frac{\partial \chi^k}{\partial y_j} \right\rangle = \frac{1}{|Y|}\int_Y (a_{ik} - a_{ij}\frac{\partial \chi^k}{\partial y_j})dy. \tag{2.31}$$

The main steps described above can be summarized as the following *homogenization procedure*:

1. Identify and solve the cell problem (2.22).
2. Insert the solution of the cell problem into (2.31) and compute the homogenized coefficients.
3. Impose appropriate boundary conditions and solve the homogenized problem (2.30).

The solution of (2.30) represents an averaged solution of the original problem (2.5) - (2.6).

Chapter 3

Numerical computation of the homogenized coefficients

3.1 Weak formulation of the cell problem

The homogenized coefficients are given by (2.31)

$$q_{ik} = \left\langle a_{ik} - a_{ij}\frac{\partial \chi^k}{\partial y_j} \right\rangle = \frac{1}{|Y|}\int_Y (a_{ik} - a_{ij}\frac{\partial \chi^k}{\partial y_j})dy. \tag{3.1}$$

In order to compute these coefficients, we need to solve the cell problem (2.22)

$$A_0\chi^k = -\frac{\partial a_{ik}}{\partial y_i}(y),\ \chi^k(y)\ Y\text{-periodic} \tag{3.2}$$

for χ^k so that we can compute the integral in (3.1). To get a weak formulation of (3.2), we note that

$$-A_0 y_k = -\left[-\frac{\partial}{\partial y_i}(a_{ij}(y)\frac{\partial}{\partial y_j})\right] y_k = \frac{\partial a_{ij}}{\partial y_i}\delta_{jk} = \frac{\partial a_{ik}}{\partial y_i}, \tag{3.3}$$

so that (3.2) can be written

$$A_0(\chi^k - y_k) = 0,\ \chi^k(y)\ Y\text{-periodic}. \tag{3.4}$$

Now we introduce the space of all Y-periodic functions in $H^1(Y)$ as

$$W(Y) = \{\Psi \in H^1(Y) : \Psi \text{ is } Y\text{-periodic }\}.$$

Assume that we have a solution $\vartheta^k = \chi^k - y_k$ to (3.4) and $\vartheta \in W(Y)$. Then we take $\zeta \in W(Y)$ and multiply it with $A_0\vartheta$ and integrate over Y to get

$$\int_Y (A_0\vartheta)\zeta dy = -\int_Y \frac{\partial}{\partial y_i}(a_{ij}(y)\frac{\partial \vartheta}{\partial y_j})\zeta dy =$$

$$= \int_Y a_{ij}(y)\frac{\partial \vartheta}{\partial y_j}\frac{\partial \zeta}{\partial y_i}dy - \oint_{\partial Y} a_{ij}(y)\frac{\partial \vartheta}{\partial y_j}\zeta n_i ds \tag{3.5}$$

by Green's theorem. We then use the fact that $a_{ij}(y)$ is Y-periodic together with Gauss' theorem (2.3) and get

$$\int_Y (A_0\vartheta)\zeta dy = \int_Y a_{ij}(y)\frac{\partial \vartheta}{\partial y_j}\frac{\partial \zeta}{\partial y_i}dy. \tag{3.6}$$

If we define $a_Y(\vartheta, \zeta)$ through

$$a_Y(\vartheta, \zeta) = \int_Y a_{ij}(y)\frac{\partial \vartheta}{\partial y_j}\frac{\partial \zeta}{\partial y_i}dy, \tag{3.7}$$

we can write the weak formulation of (3.2) as:

Find $\chi^k \in W(Y)$ such that

$$a_Y(\chi^k - y_k, \Psi) = 0 \text{ for all } \Psi \in W(Y), \tag{3.8}$$

or

Find $\chi^k \in W(Y)$ such that

$$a_Y(\chi^k, \Psi) = a_Y(y_k, \Psi) = L_Y^k(\Psi) \text{ for all } \Psi \in W(Y), \tag{3.9}$$

where

$$L_Y^k(\vartheta) = \int_Y a_{ij}(y)\frac{\partial y_k}{\partial y_j}\frac{\partial \vartheta}{\partial y_i}dy = \int_Y a_{ik}(y)\frac{\partial \vartheta}{\partial y_i}dy. \tag{3.10}$$

It should be noted that the solution of (3.8) or (3.9) is only unique up to an additive constant, as will be shown in Chapter 4.

3.2 Finite element solutions of the cell problem

In order to obtain a FEM formulation of (3.8) or (3.9), we now make a subdivision of the unit cell Y in N triangles K_n and M nodes N_i according

to Johnson [10]. Let $W_h(Y)$ be a finite-dimensional subspace of $W(Y)$ of dimension P. We introduce finite element base functions $\varphi_j(y) \in W_h(Y)$, $j = 1, 2, ..., P$, where P denotes the number of degrees of freedom. Generally, P is seldom equal to M, because in the case of Y-periodicity, nodes at opposite positions on the boundary of the Y-cell must correspond to the same degrees of freedom. To relate the nodes to the degrees of freedom, we let Q be a mapping from node N_i to the corresponding degree of freedom l, that is $l = Q(N_i)$. We also choose the base functions to be piecewise linear and define them by

$$\varphi_j(N_i) = \delta_{jl}, \text{ where } l = Q(N_i). \tag{3.11}$$

We assume an approximate solution to (3.9) of the form

$$\chi_h^k(y) = \sum_{j=1}^{P} \xi_j^k \varphi_j(y), \tag{3.12}$$

where ξ_j^k are constants to be determined. Let $\psi \in W_h(Y)$ so that ψ has the unique representation

$$\psi = \sum_{i=1}^{P} \eta_i \varphi_i. \tag{3.13}$$

We can now formulate the discrete analogue to the problem (3.9):

Find $\chi_h^k \in W_h(Y)$ such that

$$a_Y(\chi_h^k, \psi) = a_Y(y_k, \psi) = L_Y^k(\psi) \text{ for all } \psi \in W_h(Y). \tag{3.14}$$

Because (3.14) must be valid for every $\psi \in W_h(Y)$, (3.14) will be valid for $\psi = \varphi_i(y)$, $j = 1, 2, .., P$. This is mainly the idea behind the *Galerkin method*. With $\psi = \varphi_i(y)$, (3.14) becomes

$$\sum_{j=1}^{P} A_{ij} \xi_j^k = b_i^k, \ i = 1, 2, ..., P, \tag{3.15}$$

or in matrix form

$$A\xi^k = b^k, \tag{3.16}$$

where

$$A_{ij} = a_Y(\varphi_j, \varphi_i) \tag{3.17}$$

and

$$b_i^k = L_Y^k(\varphi_i). \tag{3.18}$$

In order to prove existence and uniqueness of the solutions of (3.16), we will now state some lemmas and theorems. For the matrix (A_{ij}) the following holds:

Lemma 2 *The reduced matrix obtained from the stiffness matrix A by removing row m and column m for a fixed m is positive definite.*

Proof: From the representation (3.13), we have

$$a_Y(\psi,\psi) = a_Y(\sum_{i=1}^{P}\eta_i\varphi_i, \sum_{j=1}^{P}\eta_j\varphi_j) = \sum_{i=1}^{P}\sum_{j=1}^{P}\eta_i a_Y(\varphi_i,\varphi_j)\eta_j = \eta\cdot A\eta,$$

where the dot denotes the usual scalar product in $\mathbf{R}^P$. But we also have, recalling (2.4), that a_{ij} is positive definite, and hence

$$\eta\cdot A\eta = a_Y(\psi,\psi) = \int_Y a_{ij}\frac{\partial\psi}{\partial y_j}\frac{\partial\psi}{\partial y_i}dy \geq \alpha\int_Y |\nabla\psi|^2\, dy \geq 0$$

with equality if and only if $\nabla\psi \neq 0$, that is, if

$$\psi(y) = \sum_{i=1}^{P}\eta_i\varphi_i(y) = C_\eta,\ C_\eta\ constant.$$

By the definition of φ_i, this holds only if

$$\eta_1 = \eta_2 = ... = \eta_P = C_\eta.$$

Now fix $\eta_1 = 0$. Then

$$\sum_{i=1}^{P}\sum_{j=1}^{P}\eta_i a_Y(\varphi_i,\varphi_j)\eta_j = \sum_{i=2}^{P}\sum_{j=2}^{P}\eta_i a_Y(\varphi_i,\varphi_j)\eta_j = 0$$

if and only if

$$\eta_2 = \eta_3 = ... = \eta_P = 0.$$

Hence the reduced matrix obtained by removing row 1 and column 1 is positive definite. The above procedure can be done on any row and column m so the lemma follows.

We now need the following definition and lemma:

Definition 3 *A positive cone in a real linear space is a subset M with the property that if $u \in M$, then $\alpha u \in M$ for all real numbers $\alpha \geq 0$.*

Lemma 4 *(Poincaré inequality version 1): Let Ω be an open, bounded and connected set in $\mathbf{R}^n$ with the Lipschitz property and let M be a closed positive cone of $H^1(\Omega)$, not containing the constant functions $\neq 0$. Then*

$$\int_\Omega |u|^2 \, dx \leq C \int_\Omega \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_i} dx = C \int_\Omega |\nabla u|^2 \, dx \tag{3.19}$$

for all $u \in M$ and some constant $C = C(\Omega)$.

Proof: See e.g. Alt [1], p. 170-171.

If we assume that ϑ is not a nonzero constant function, we can state the following inequalities:

Lemma 5 *The following statements holds true for the bilinear form $a_Y(\vartheta, \zeta)$ and the linear functional $L_Y^k(\vartheta)$ if ϑ is not a nonzero constant function.*

1. *$a_Y(\vartheta, \zeta)$ is coercive, that is, there is a constant $\beta > 0$ such that*

$$a_Y(\vartheta, \vartheta) \geq \beta \left\| \vartheta \right\|_{W(Y)}^2, \, \forall \vartheta \in W(Y). \tag{3.20}$$

2. *$L_Y^k(\vartheta)$ is bounded, that is, there is a constant $\Lambda > 0$ such that*

$$\left| L_Y^k(\vartheta) \right| \leq \Lambda \left\| \vartheta \right\|_{W(Y)}, \forall \vartheta \in W(Y). \tag{3.21}$$

Proof: 1. First we note that $W(Y)$ is a closed positive cone of $H^1(\Omega)$, then we use the Poincaré inequality together with (2.4) and get

$$a_Y(\vartheta, \vartheta) = \int_Y a_{ij}(y) \frac{\partial \vartheta}{\partial y_j} \frac{\partial \vartheta}{\partial y_i} dy \geq \int_Y \alpha \frac{\partial \vartheta}{\partial y_i} \frac{\partial \vartheta}{\partial y_i} dy \geq$$

$$\geq \frac{\alpha}{1 + C} \int_Y |\vartheta|^2 + |\nabla \vartheta|^2 \, dy = \beta \left\| \vartheta \right\|_{W(Y)}^2,$$

where $\beta = \frac{\alpha}{1+C}$. 2. We use Schwartz' inequality on (3.10) and get

$$\left| L_Y^k(\vartheta \right| = \left| \int_Y a_{ik} \frac{\partial \vartheta}{\partial y_i} dy \right| \leq \left\| a_{ik} \right\|_{L^\infty(Y)} \int_Y \left| \frac{\partial \vartheta}{\partial y_i} \right| dy \leq$$

$$\leq \left\| a_{ik} \right\|_{L^\infty(Y)} \left\| \frac{\partial \vartheta}{\partial y_i} \right\|_{L^2(Y)} \left\| 1 \right\|_{L^2(Y)} \leq \Lambda \left\| \vartheta \right\|_{W(Y)},$$

where $\Lambda = \left\| a_{ik} \right\|_{L^\infty(Y)} |Y|$.

Theorem 6 *There exists a unique solution $\xi^k \in \mathbf{R}^P$ to the problem (3.15) if we fix for instance $\xi_1^k = 0$. This means that there exists a unique solution $\chi_h^k \in W_h(Y)$ to (3.14). Moreover, the following stability estimate holds:*

$$\left\|\chi_h^k\right\|_{W(Y)} \leq \frac{\Lambda}{\beta} \tag{3.22}$$

Proof: Lemma 2 says that A is positive definite if we for instance fix $\xi_1^k = 0$. Hence A is non-singular, which proves existence and uniqueness. Fixing one $\xi_i^k = 0$ for some number i means that the only possible constant function χ_h^k is $\chi_h^k = 0$. The stability estimate follows by choosing $\psi = \chi_h^k$ in (3.14) which gives, using (3.20) and (3.21),

$$\beta \left\|\chi_h^k\right\|_{W(Y)}^2 \leq a_Y(\chi_h^k, \chi_h^k) = L_Y^k(\chi_h^k) \leq \Lambda \left\|\chi_h^k\right\|_{W(Y)},$$

(no summation over k), from which (3.22) follows upon division by $\beta \left\|\chi_h^k\right\|_{W(Y)}$ $\neq 0$.

We can now compute the approximate homogenized coefficients by insert (3.12) in (3.1) to get

$$q_{ik} = \frac{1}{|Y|}\int_Y (a_{ik} - a_{ij}\sum_{l=1}^P \xi_l^k \frac{\partial \varphi_l}{\partial y_j})dy =$$

$$= \frac{1}{|Y|}\int_Y a_{ik}dy - \frac{1}{|Y|}\sum_{l=1}^P \xi_l^k \int_Y a_{ij}\frac{\partial \varphi_l}{\partial y_j}dy. \tag{3.23}$$

We now note that

$$a_Y(\varphi_l, y_i) = \int_Y a_{mj}\frac{\partial \varphi_l}{\partial y_j}\frac{\partial y_i}{\partial y_m}dy = \int_Y a_{ij}\frac{\partial \varphi_l}{\partial y_j}dy, \tag{3.24}$$

because $\frac{\partial y_i}{\partial y_m} = \delta_{im}$ and hence

$$q_{ik} = \frac{1}{|Y|}\int_Y a_{ik}dy - \frac{1}{|Y|}\sum_{l=1}^P a_Y(\varphi_l, y_i)\xi_l^k. \tag{3.25}$$

If a_{ik} is symmetric, (3.10) and (3.18) gives

$$\int_Y a_{ij}\frac{\partial \varphi_l}{\partial y_j}dy = \int_Y a_{ji}\frac{\partial \varphi_l}{\partial y_j}dy = L_Y^i(\varphi_l) = b_l^i \tag{3.26}$$

so that

$$q_{ik} = \frac{1}{|Y|}\int_Y a_{ik}dy - \frac{1}{|Y|}\sum_{l=1}^P b_l^i \xi_l^k. \tag{3.27}$$

Chapter 4

Existence and uniqueness of weak solutions for elliptic problems

In this section, we will prove existence and uniqueness of weak solutions of the boundary value problems considered in the previous sections. Moreover, we will prove Lemma 1 and some properties of the homogenized coefficients. To prove this, we will need another version of the *Poincaré inequality* and the *Lax-Milgram lemma:*

Definition 7 *Let X be a real Hilbert space. A mapping*

$$a(\cdot,\cdot) : X \times X \to \mathbf{R}$$

is called a bilinear form on X if

1. $a(x_1 + x_2, y) = a(x_1, y) + a(x_2, y)$ *for all* $x_1, x_2, y \in X$,
2. $a(\alpha x, y) = \alpha a(x, y)$ *for all* $x, y \in X$ *and* $\alpha \in \mathbf{R}$,
3. $a(x, y_1 + y_2) = a(x, y_1) + a(x, y_2)$ *for all* $x, y_1, y_2 \in X$,
4. $a(x, \beta y) = \beta a(x, y)$ *for all* $x, y \in X$ *and* $\beta \in \mathbf{R}$.

Definition 8 *Let $a(\cdot,\cdot)$ be a bilinear form on the real Hilbert space X. We say that $a(\cdot,\cdot)$ is*

1. *bounded if there exists a constant* $\gamma > 0$ *such that* $|a(x,y)| \leq \gamma \|x\|_X \|y\|_X$ *for all* $x, y \in X$.

2. *symmetric if* $a(x,y) = a(y,x)$ *for all* $x, y \in X$.

3. *coercive if there exists a constant* $\alpha > 0$ *such that* $a(x,x) \geq \alpha \|x\|_X^2$ *for all* $x \in X$.

Lemma 9 *(Poincaré inequality version 2): Let* Ω *be an open and bounded set in* $\mathbf{R}^n$ *which has the Lipschitz property. Then*

$$\|u\|^2_{H^1(\Omega)/\mathbf{R}} \leq C \int_\Omega \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_i} dx \tag{4.1}$$

for each $u \in H^1(\Omega)/\mathbf{R}$ *and some constant* $C = C(\Omega)$.

Proof: See e.g. Necas [14].

Lemma 10 *(Lax-Milgram): Let* X *be a real Hilbert space. If the bilinear form* $a(\cdot,\cdot) : X \times X \to \mathbf{R}$ *is bounded and coercive and if, in addition, the linear functional* $f : X \to \mathbf{R}$ *is bounded, then there exists a unique element* $x \in X$ *such that* $a(x,y) = (f,y)$ *for all* $y \in X$.

Proof: See e.g. Alt [1], p. 118-119.
We recall equations (2.1) and (2.2), that is,

$$-\frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right) = f(x) \text{ in } \Omega, \tag{4.2}$$

$$u = 0 \text{ on } \Gamma_1 \text{ and } a_{ij}(x)\frac{\partial u}{\partial x_j} n_i = g \text{ on } \Gamma_2, \tag{4.3}$$

where $\Gamma_1 \cup \Gamma_2 = \partial\Omega$ and $\Gamma_1 \cap \Gamma_2 = \emptyset$. We assume that

- $a_{ij} \in L^\infty(\Omega)$,
- a_{ij} is positive definite, that is, $a_{ij}(y)\xi_i\xi_j \geq \alpha\xi_i\xi_i$ almost everywhere for some constant $\alpha > 0$ and all $\xi \in \mathbf{R}^n$,
- $f \in L^2(\Omega)$ and $g \in L^2(\Gamma_2)$.

We define $V = \{v \in H^1(\Omega) : v|_{\Gamma_1} = 0\}$ and note that $H_0^1(\Omega) \subset V \subset H^1(\Omega)$. Furthermore, we define the bilinear form

$$a(u,v) = \int_\Omega a_{ij}(x) \frac{\partial u}{\partial x_j} \frac{\partial v}{\partial x_i} dx \tag{4.4}$$

and the linear functional

$$L(v) = \int_\Omega f v dx + \int_{\Gamma_2} g v dS. \tag{4.5}$$

The weak formulation of (2.1) and (2.2) takes the following form:

Find $u \in V$ such that

$$a(u,v) = L(v) \text{ for all } v \in V \tag{4.6}$$

This follows by multiplying each side of (2.1) by a function $v \in V$, integrating over Ω and applying Gauss' theorem on the left hand side. We have the following theorem:

Theorem 11 *Let Ω be an open, bounded and connected set in $\mathbf{R}^n$ with the Lipschitz property. Then*

1. *If Γ_1 has strictly positive surface measure, then there exists a unique solution $u \in V$ of equation (4.6).*
2. *If Γ_1 has surface measure zero, then there exists a solution $u \in V$ of equation (4.6). This solution is unique up to an additive constant.*

Proof: (i): V is a closed subspace of $H^1(\Omega)$ by the trace theorem (see e.g. Alt [1], p. 190). In particular, V is a closed positive cone in $H^1(\Omega)$ and the boundary condition implies that V contains no other constant functions than $u \equiv 0$. Thus Lemma 4 and the positiveness of a_{ij} yield

$$\alpha_1 \|v\|_V^2 \leq a(v,v)$$

for some positive constant α_1. Furthermore, the bilinear form is bounded, since, by Schwarz inequality,

$$|a(u,v)| \leq \|a_{ij}\|_{L^\infty} \left(\left\| \frac{\partial u}{\partial x_i} \right\|_{L^2}^2 \right)^{\frac{1}{2}} \left(\left\| \frac{\partial u}{\partial x_j} \right\|_{L^2}^2 \right)^{\frac{1}{2}} \leq C_0 \|u\|_V \|v\|_V$$

for some positive constant C_0. Finally, $L(v)$ is a bounded linear functional since, by using the Schwarz' inequality once again and by using the trace theorem, we obtain

$$L(v) \leq C \|f\|_{L^2} \|v\|_V + C_1 \|g\|_{L^2(\Gamma_2)} \|v\|_V$$

for some positive constants C and C_1. Therefore, we can apply the Lax-Milgram lemma and conclude that there exists a unique solution $u \in V$ of equation (4.6).

(ii): Here, $V = H^1(\Omega)$. In this case $a(\cdot,\cdot)$ is not coercive in $H^1(\Omega)$ in general and therefore we consider the quotient space $H^1(\Omega)/\mathbf{R}$. By using Lemma 9, we conclude that $a(\cdot,\cdot)$ is coercive in $H^1(\Omega)/\mathbf{R}$. We proceed as in the proof of (i) and find that there exists a unique function $u \in H^1(\Omega)/\mathbf{R}$, which is a solution of equation (4.6). Finally, uniqueness in $H^1(\Omega)/\mathbf{R}$ means uniqueness up to an additive constant and the theorem is proved.

We now restate Lemma 1 from Chapter 2 in order to prove it:

Lemma 12 *Let F be square integrable over Y and consider the boundary value problem*

$$A_0\Phi = F \text{ in a unit } Y\text{-cell, } \Phi \text{ is } Y\text{-periodic.} \tag{4.7}$$

The following holds true:

1. *There exists a weak Y-periodic solution Φ of (4.7) if and only if $\langle F \rangle = 0$.*
2. *If there exists a weak Y-periodic solution of (4.7), then it is unique up to an additive constant.*

Proof: We introduce the Hilbert space

$$W(Y) = \{\Psi \in H^1(Y) : \Psi \text{ is } Y\text{-periodic}\},$$

the bilinear form

$$a_Y(\Phi, \Psi) = \int_Y a_{ij} \frac{\partial \Phi}{\partial y_j} \frac{\partial \Psi}{\partial y_i} dy$$

and the linear functional

$$(F, \Psi)_Y = \int_Y F\Psi dy.$$

Then the weak formulation of (4.7) is:

Find $\Phi \in W(Y)$ such that

$$a_Y(\Phi, \Psi) = (F, \Psi)_Y \text{ for all } \Psi \in W(Y) \tag{4.8}$$

Assume that Φ is a solution and choose $\Psi \equiv 1$. Then

$$0 = a_Y(\Phi, 1) = (F, 1) = |Y| \langle F \rangle ,$$

which shows that $\langle F \rangle = 0$. Conversely, assume that $\langle F \rangle = 0$. It is clear that the bilinear form $a_Y(\Phi, \Psi)$ is not coercive in $W(Y)$, since if Ψ is a nonzero constant function, then $a_Y(\Psi, \Psi) = 0$ but $\|\Psi\|_{W(Y)} > 0$. However, according to Lemma 9, it is coercive in $W(Y)/\mathbf{R}$. Moreover, since a_{ij} is bounded, it follows that $a_Y(\cdot, \cdot)$ is bounded in $W(Y)/\mathbf{R}$. $(F, \Psi)_Y$ is a well-defined continuous linear functional on $W(Y)/\mathbf{R}$, since if c is a constant,

$$\int_Y F c dy = c \int_Y F dy = c\,|Y| \langle F \rangle = 0$$

and therefore

$$(F, \Psi)_Y = \int_Y F \Psi dy = \int_Y F(\Psi - c) dy.$$

Hence

$$|(F, \Psi)_Y| \leq \|F\|_{L^2(Y)} \inf_{c \in \mathbf{R}} \|\Psi - c\|_{L^2(Y)} \leq \|F\|_{L^2(Y)} \|\Psi\|_{W(Y)/\mathbf{R}} .$$

Now, by the Lax-Milgram lemma, there exists a unique solution Φ in $W(Y)/\mathbf{R}$ to (4.8). But uniqueness in $W(Y)/\mathbf{R}$ means uniqueness up to an additive constant in $W(Y)$ and the lemma is proved.

We finally prove some properties of the homogenized tensor $q_{ij.}$

Theorem 13 *Let a_{ij} be a symmetric and positive definite tensor. Then the associated homogenized tensor q_{ij}, defined as in (2.31), is symmetric and positive definite.*

Proof: We consider the cell problem (2.22) and recall the weak formulation (3.8):

Find $\chi^k \in W(Y)$ such that

$$a_Y(\chi^k - y_k, v) = 0 \tag{4.9}$$

for all $v \in W(Y)$, where $W(Y)$ and $a_Y(\cdot,\cdot)$ are defined as earlier. According to (2.31), we have

$$q_{ik} = \frac{1}{|Y|}\int_Y (a_{ik} - a_{ij}\frac{\partial \chi^k}{\partial y_j})dy = \frac{1}{|Y|}\int_Y (a_{mj}\delta_{jk}\delta_{im} - a_{mj}\delta_{im}\frac{\partial \chi^k}{\partial y_j})dy =$$

$$= \frac{1}{|Y|}\int_Y (a_{mj}\frac{\partial y_k}{\partial y_j}\frac{\partial y_i}{\partial y_m} - a_{mj}\frac{\partial \chi^k}{\partial y_j}\frac{\partial y_i}{\partial y_m})dy =$$

$$= \frac{1}{|Y|}\int_Y a_{mj}(\frac{\partial \chi^k}{\partial y_j} - \frac{\partial y_k}{\partial y_j})\left(-\frac{\partial y_i}{\partial y_m}\right)dy = \frac{1}{|Y|}a_Y(\chi^k - y_k, -y_i), \qquad (4.10)$$

which, by using (4.9) with $v = \chi^i$, gives

$$q_{ik} = q_{ik} + 0 = \frac{1}{|Y|}a_Y(\chi^k - y_k, -y_i) + \frac{1}{|Y|}a_Y(\chi^k - y_k, \chi^i) =$$

$$= \frac{1}{|Y|}a_Y(\chi^k - y_k, \chi^i - y_i). \qquad (4.11)$$

If $a_{ij} = a_{ji}$, then $a_Y(u,v) = a_Y(v,u)$ and hence, by (4.11), $q_{ik} = q_{ki}$, that is, q_{ik} is symmetric.

Now we consider $q_{ik}\xi_i\xi_k$ for an arbitrary $\xi \in \mathbf{R}^n$. Let $\omega = \xi_i(\chi^i - y_i)$. The positive definiteness of a_{ij} and (4.11) yield

$$q_{ik}\xi_i\xi_k = \frac{1}{|Y|}a_Y(\omega,\omega) \geq \alpha\left\langle \frac{\partial \omega}{\partial y_i}\frac{\partial \omega}{\partial y_i}\right\rangle \geq 0. \qquad (4.12)$$

Thus, $q_{ik}\xi_i\xi_k \geq 0$ with equality if and only if $\frac{\partial \omega}{\partial y_i} = 0$, that is, if and only if $\omega \equiv c$ (constant), or equivalently, $\xi_i y_i = \xi_i\chi^i - c$. Here χ^i is Y-periodic so that equality holds if and only if $\xi_i = 0$, and the theorem is proved.

Chapter 5

Numerical results

5.1 The computer program

To compute the homogenized coefficients, we developed a finite element computer program with integrated homogenization routines. Some of the specifications of the program were that it should be *demonstrative, compact* and *easy to use.* To achieve this, we wrote the computer program in the programming language *Turbo Pascal 7.0* by *Borland International Inc.*

The program has routines for the construction of both quadratic and hexagonal unit cells and it automatically triangulates these unit cells with respect to the chosen volume percentage of material 2. If some other type of unit cell is wanted, the program has an entering/editing command, with which one can manually construct and triangulate any type of unit cell. Moreover, if one wants to edit a unit cell in some other editor, the program has loading and saving facilities. After a unit cell is constructed, the user is asked to enter the conductivity tensor. When this is done, the program can now solve the equations from the finite element formulation of the problem, and with some integration routines compute the effective conductivities. The result is then compared with some known bounds, and the user can also plot the solutions of the cell problem on the screen. The major advantage of this program is that it does every step of the homogenization procedure. This is in general not possible in commercial FEM programs, and moreover, they do in general not support periodic boundary conditions, which is a large obstacle when computing homogenized coefficients.

The source code is called EffCond.PAS and the executable, compiled code

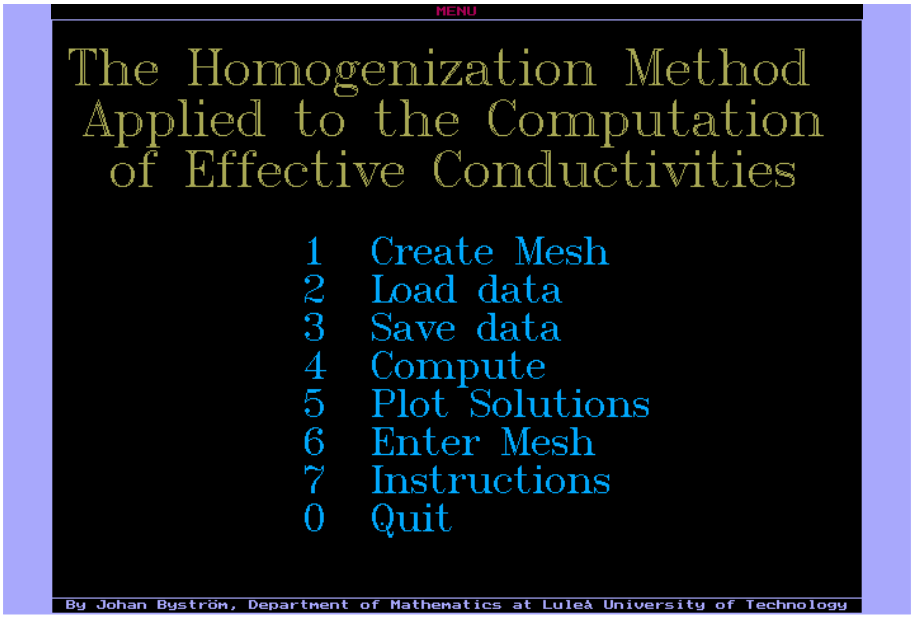


Figure 5.1: The main menu of the computer program.

is called EffCond.EXE and can be accessed by contacting us. The program is written for any PC-type computer with at least VGA graphics. If existent, the program will make use of the *80X87* floating point coprocessor for extra speed. The program is mainly composed of six parts:

(a) Input of data.
(b) Construction and representation of the triangulation T_h.
(c) Computation of the element stiffness matrices a^{K_n} and element loads $b^{K_n}(k)$.
(d) Assembly of the global stiffness matrix A and load vectors $b(k)$.
(e) Solution of the systems of equations.
(f) Presentation of the results.

5.1.1 Input of data

The input data are:

(a) Type of unit cell, quadratic or hexagonal.
(b) Volume fraction of material 2, that is volume fraction of fibres.
(c) Fineness of mesh.
(d) Conductivity tensor.

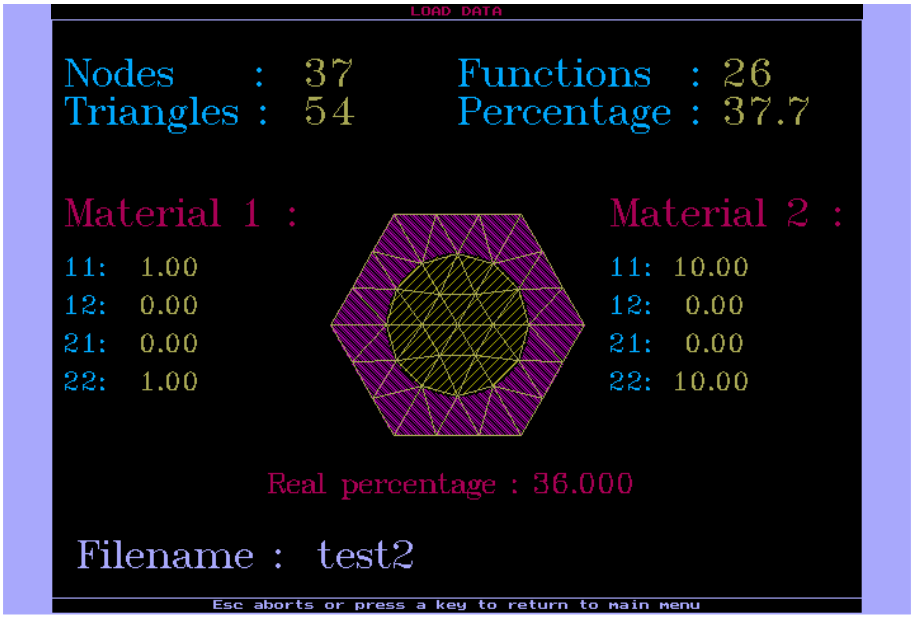


Figure 5.2: A hexagonal unit cell loaded from the file *test2.dat*.

The program has an interactive interface, which enables the user to enter the above data. The data can also be loaded from a file, see Figure 5.2. The result is a triangulated unit cell, ready for computation.

5.1.2 Construction and representation of the triangulation

When the above data has been entered, the program triangulates the unit cell automatically and with respect to the chosen volume fraction, see Figure 5.3. The given triangulation T_h is represented as follows: Let N_i, $i = 1, ..., M$, and K_n, $n = 1, ..., N$ be enumerations of the nodes and triangles of T_h, respectively. Then T_h may be specified using the two arrays $Z : 2 \times M$ and $T : 3 \times N$, where $Z(j, i)$, $j = 1, 2$ are the coordinates of node N_i and $T(j, n)$, $j = 1, 2, 3$, are the numbers of the vertices of triangle K_n. Because of the Y-periodicity, nodes on opposite sides of the cell will have equal value. Therefore, there will be P base functions and $P < M$. We therefore need a mapping Q from the node N_i to the degree of freedom l, that is $l = Q(N_i)$.

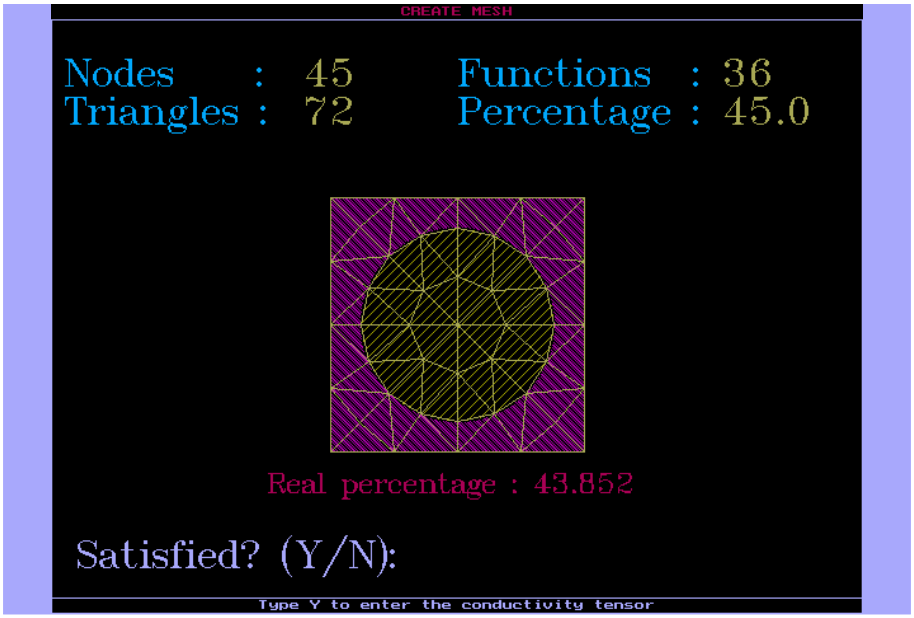


Figure 5.3: A triangulated quadratic unit cell.

In practice, this mapping is a matrix $Q : 1 \times M$ where Q_i denotes the degree of freedom for node N_i. Because the unit cell is divided into two parts with different conductivity tensors, we also need a matrix $\lambda : 1 \times N$, where $\lambda_n = 1$ if the triangle K_n covers material 1 and $\lambda_n = 2$ if the triangle K_n covers material 2. The triangulation is now fully represented by these four matrices.

5.1.3 Computation of the element stiffness matrices a^{K_n} and element loads $b^{K_n}(k)$

We now compute the so called element stiffness matrices a^{K_n} and element loads $b^{K_n}(k)$. These matrices and vectors are the stiffness matrices and load vectors of triangle K_n. We know that $a_{ij}^{K_n} \neq 0$ only if both N_i and N_j are nodes of K_n. We have that $T(\alpha, n)$, $\alpha = 1, 2, 3$, are the numbers of the vertices of K_n, and the x_i-coordinates, $i = 1, 2$, for these vertices are given by $Z(i, T(\alpha, n))$. Knowing the vertices of K_n we can now compute the element stiffness matrix $A^{K_n} = (a_{\alpha\beta}^{K_n})$, $\alpha, \beta = 1, 2, 3$, and the element load vectors

$b^{K_n}(k) = (b_\alpha^{K_n}(k))$, $\alpha = 1, 2, 3$, for element K_n as

$$a_{\alpha\beta}^{K_n} = \int_{K_n} a_{ij} \frac{\partial \psi_\alpha}{\partial y_j} \frac{\partial \psi_\beta}{\partial y_i} dy \tag{5.1}$$

and

$$b_\alpha^{K_n}(k) = \int_{K_n} a_{ik} \frac{\partial \psi_\alpha}{\partial y_i} dy, \ k = 1, 2. \tag{5.2}$$

where ψ_α is the linear function on K_n that takes on the following values:

$$\psi_\alpha(N_{T(\beta,n)}) = \delta_{\alpha\beta}, \ \alpha, \beta = 1, 2, 3. \tag{5.3}$$

These integrals can be computed by for instance Gauss quadrature, but because we work with piecewise linear functions, we will integrate a constant over a triangle K_n. This means that we can compute the integrals by first computing the area of triangle K_n by Heron's formula and then multiply it with the constant value to get the integrals.

Thus, we then compute the $3\times$ 3 matrix A^{K_n} and the two 1×3 vectors $b^{K_n}(k)$ for all triangles K_n and then proceed to assemble the global stiffness matrix.

5.1.4 Assembly of global stiffness matrix and load vectors

To assemble the global stiffness matrix $A = (A_{ij})$ and the load vectors $b(k)$ we just loop over all elements K_n and successively add in the contributions from different K_n as follows:

Set $A_{ij} = 0$, $b_i(1) = 0$, $b_i(2) = 0$, $i, j = 1, ..., P$
For $n = 1, ..., N$ set
$A_{Q(T(\alpha,n)),Q(T(\beta,n))} = A_{Q(T(\alpha,n)),Q(T(\beta,n))} + a_{\alpha\beta}^{K_n}$
$b_{Q(T(\alpha,n))}(k) = b_{Q(T(\alpha,n))}(k) + b_\alpha^{K_n}(k)$, $k = 1, 2$ for $\alpha, \beta = 1, 2, 3$.

5.1.5 Solution of the linear systems

To solve the linear systems, we use the Gauss-Seidel iteration method as described in Kincaid and Cheney [11], p. 230-231. We start with the zero vector and thereby automatically fixes one of the components to zero. Hence the iteration converges to a solution, while the stiffness matrix is positive definite.

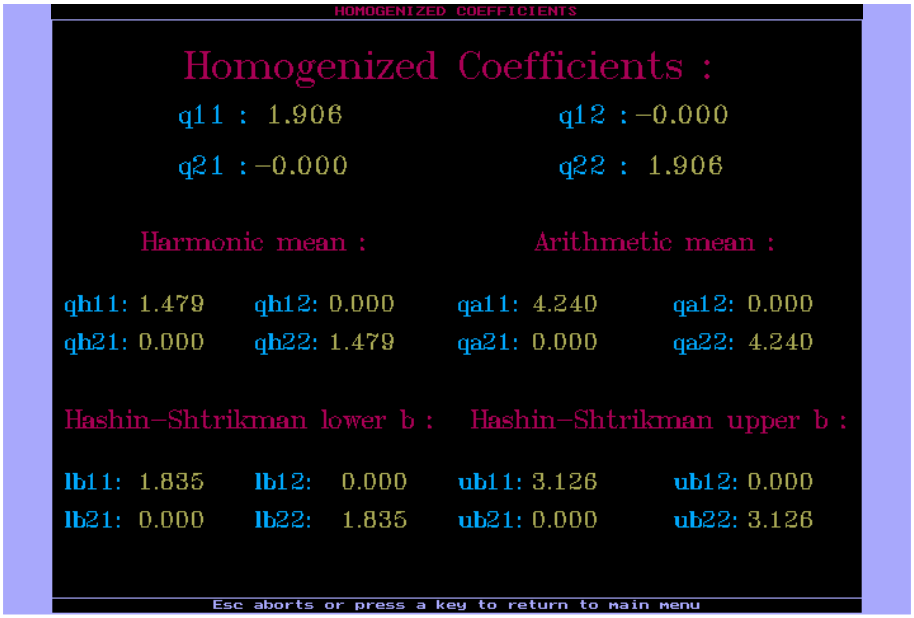


Figure 5.4: The computed coefficients compared with various bounds.

5.1.6 Presentation of the results

Finally, the results of the computations are presented in two different ways. First, the computed coefficients are presented together with the *arithmetic mean* and the *harmonic mean* (also known as the *Reuss-Voigt bounds*), and the upper and lower *Hashin-Shtrikman bounds*, see Figure 5.4.

Second, the solutions are plotted on the screen, to show for instance where the biggest gradient errors occur, see Figure 5.5.

5.2 A comparison of computed coefficients with various bounds

We used the program to compute some effective conductivities q and to compare them with previous results (Persson [16]) and also to compare them with the different bounds that exist. If $\nu_1$denotes the volume fraction of material 1 with heat conductivity λ_1 and ν_2 denotes the volume fraction of material 2 with heat conductivity λ_2, it can be shown (see e.g. Attouch [2])



Figure 5.5: The solution of the cell problem plotted for a quadratic unit cell.

that

$$M_h \leq q \leq M_a,$$

where M_h denotes the harmonic mean

$$M_h = \frac{1}{\frac{\nu_1}{a_2} + \frac{\nu_2}{\lambda_2}} \tag{5.4}$$

and M_a denotes the arithmetic mean

$$M_a = \nu_1\lambda_1 + \nu_2\lambda_2. \tag{5.5}$$

However, there are even stronger bounds, the so called Hashin-Shtrikman bounds (Wendt et al. [20], p. 232-233). If $\lambda_1 < \lambda_2$, they are defined through

$$q^- = \lambda_1 + \frac{\nu_2}{\frac{1}{\lambda_2-\lambda_1} + \frac{\nu_1}{2\lambda_1}}, \tag{5.6}$$

$$q^+ = \lambda_2 + \frac{\nu_1}{\frac{1}{\lambda_1-\lambda_2} + \frac{\nu_2}{2\lambda_2}} \tag{5.7}$$

so that

$$q^- \leq q \leq q^+.$$

We computed some homogenized heat conductivities using a quadratic and a hexagonal unit cell. We used 72 elements in the quadratic unit cell and 54 elements in the hexagonal unit cell. We now present these numerical results and compare them with the bounds and with earlier computed values by Persson [16].

λ_1	1.0	1.0	1.0	1.0
λ_2	10.0	23.1	29.8	29.8
ν_2	0.25	0.64	0.50	0.35
q_{Quad}	1.574	4.449	2.948	2.075
q_{Hex}	1.579	4.068	2.896	2.078
q_h	1.290	2.579	1.935	1.511
q_a	3.250	15.14	15.40	11.08
q_{low}	1.514	3.841	2.756	1.973
q_{high}	2.394	11.63	10.81	7.269
q_{Comp}	1.516	4.224	2.871	1.981

In this table, q_{Quad} and q_{Hex} denotes computed q for quadratic and hexagonal unit cells, respectively. We compare those values with q_h, q_a, q_{low}, q_{high} and q_{Comp}, where q_h and q_a are the harmonic and arithmetic means, q_{low} and q_{high} are the lower and upper Hashin-Shtrikman bounds, and finally, q_{Comp} are the earlier computed values by Persson [16].

5.2.1 Discussion

We see that the quadratic unit cell gives slightly higher values than the hexagonal unit cell. This is much because of the finer mesh of the quadratic unit cell. The difference grows when the percentage of material 2 grows. This is because there is a bigger overlap in the boundary between the both materials when the fibre radius is big, that is when the volume fraction of material 2 is high. In spite of those discretization errors, the difference between the q-values are relatively small, and if we compare with the means or the Hashin-Shtrikman bounds, the difference is very small. We also note that the computed values are very similar to those of Persson [16], but our conductivities are in general higher.

Chapter 6

Some concluding words

During the last twentyfive years there has been an increasing interest in questions related to convergence of differential operators and variational convergences.

On reason for this increased interest in variational convergences is of course the possible applications to different fields of importance especially for applications. We here just mention fields such as numerical analysis, phase transitions, perturbation problems or optimal control.

In this thesis, we have presented another important application, *homogenization theory*. The field of composite media and homogenization theory is broad. A large number of papers and books, contributing to the development of the theory and to its applications, have been written, most of them during the last twentyfive years. Early contributions to homogenization goes back to Maxwell and Einstein (see e.g. Babuska [3] and [4] and Dal Maso [7] and the references given there) who considered for example effective properties for viscous fluids having spherical particles distributed. Let us also mention early contributions to the concept of lower semicontinuity and convexity by Tonelli (see e.g. Dal Maso [7] and the references given there).

For a self-contained presentation of homogenization with applications we refer to the books by Attouch [2], Bakhvalov et al. [5], Bensoussan et al. [6], Dal Maso [7], Ene et al. [8] and Sanchez-Palencia [17], where, in particular, [7] contains more than 1100 references in this connection.

We also mention the doctoral theses by Holmbom [9], Lukkassen [12] and Svanstedt [18], and the licentiate thesis by Wall [19], all of them produced by the group in homogenization at the Department of Mathematics at Luleå University of Technology.

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