An inverse homogenization design method for stress control in composites

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AN INVERSE HOMOGENIZATION DESIGN METHOD FOR STRESS CONTROL IN COMPOSITES

A Dissertation
Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
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in
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by
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Abstract

This thesis addresses the problem of optimal design of microstructure in composite materials. The work involves new developments in homogenization theory and numerical analysis. A computational design method for grading the microstructure in composite materials for the control of local stress in the vicinity of stress concentrations is developed. The method is based upon new rigorous multiscale stress criteria connecting the macroscopic or homogenized stress to local stress fluctuations at the scale of the microstructure. These methods are applied to three different types of design problems. The first treats the problem of optimal distribution of fibers with circular cross section inside a long shaft subject to torsion loading. The second treats the same problem but now the shaft cross section is filled with locally layered material. The third one treats the problem of composite design for a flange fixed at one end and loaded at the other end.
1. Introduction

Composite materials are used for a wide variety of applications. These structural materials provide high stiffness and strength properties per unit weight. By choosing an appropriate combination of reinforcement and matrix material, properties can be tailored that exactly fit the requirements for a particular structure for a particular purpose. In modern aviation it is common now to find wing and tail sections, propellers and rotor blades made from advanced composites, along with much of the internal structure and fittings. These materials are used in geometries that involve abrupt dimensional changes within structural components, such as thin structural skin connected to ribs, panel reinforcement, and junctions of struts. Associated with these geometries are stress concentrations which present a potential source for structural failure.

In this treatment we consider composite design problems that require pointwise constraints on the local stress. Any attempt to design composite microgeometry by directly optimizing over the microstructure is hopelessly complicated. Instead our approach is to introduce homogenized design variables that capture gross features of the microgeometry such as local volume fraction of fibers or fiber orientation. We then develop methods for optimizing over these variables. Finally, we use these to construct an explicit microstructure with desirable structural properties. The approach is in essence of an inverse method that uses new tools from homogenization theory to identify optimal graded microstructures. Because of this we will refer to it as an inverse homogenization design method. The design variables that we use are based upon effective elastic properties and other effective properties that measure the local stress in a composite structure.

It is now well known that effective macroscopic constitutive properties relating average stress to average strain can be used in the numerical design of composite structures for optimal structural compliance. This type of design problem has received significant attention from both the applied mathematics and structural optimization communities in the 1980s and 1990s, see for example [1], [3], [7], [8], [9], [12], [23], [24], [26], [30]. In the context of functionally graded materials this design strategy for optimizing structural properties appears in [25], [28]. In all of these works the problem of determining the optimal spatial dependence for the composition is obtained through the use of effective macroscopic constitutive relations.

Recent efforts have initiated the development of numerical methods for structural optimization in the presence of stress constraints. The problem of design of long fiber reinforced shafts for maximum torsional rigidity in the presence of mean square stress constraints has been addressed in [14]. A rigorous inverse homogenization method for the optimal distribution of fiber diameters across the shaft is developed. It is shown that the appropriate homogenized problem requires the use of the second moment or covariance tensor in addition to the effective compliance. Very recently, a homogenization method for topology design subject to mean square stress constraints using locally layered microstructures of arbitrary rank has been developed [2].

In all of the aforementioned work the stress constraints were of mean square type. In this work a rigorous design methodology is presented that allows for tighter control of local stresses at the level of the microstructure. This is important when designing against failure initiation. In what follows we provide a new methodology that delivers graded materials that provide pointwise control of the stress inside subdomains with boundaries that do not intersect the boundary of the structure. In order to proceed new macroscopic properties beyond effective constitutive laws and covariance tensors are required. In this thesis we make use of the macrofield modulation functions and the homogenization constraints given in [15], [16] and [18]. We also extend these quantities to the case of layered microstructures. The
macrofield modulation functions together with effective constitutive relations are used here to construct a suitable homogenized design problem that satisfies the two requirements associated with the inverse homogenization design method.

The goal of the design problems is to identify a graded distribution of microstructure such that the following requirements are met:

1. The reinforced structural component has a high resistance against loads.

2. The magnitude of the local pointwise stress inside the composite structure is controlled over a designated subset of the design domain.

The thesis is organized as follows: In chapter two we give a short introduction to linear elasticity. The equations and formulas of elastic equilibrium in three dimensions are given. The application of these equations to two dimensional problems of plane strain, plane stress, and torsional rigidity are provided. In chapter three the problem of reinforcement of a long shaft with constant cross section is described. The microstructure within the shaft consists of long reinforcement fibers of circular cross section embedded in a more compliant material. A constraint is placed on the total cross sectional area occupied by the fibers. In the following a suitable homogenized design problem is described. the homogenized formulation makes use of a multiscale stress criterion given in terms of the macrostress modulation functions. A gradient based numerical implementation of the inverse homogenization design method is then described and computational results are given for an “X” shaped shaft cross section.

Chapter four addresses inverse homogenization and design of locally layered microstructure for pointwise stress control. The numerical examples are carried out for “L” shaped and “X” shaped shaft cross sections. These geometries typify the junctions between composite substructures and possess reentrant corners typically seen in lap joints and junctions of struts.

In chapter five we illustrate a plane strain design problem. Here a composite flange which is fixed on one side is subjected to a load and the material is optimized for resistance against the load while at the same time keeping the stresses sufficiently low.

The derivations of the homogenization formulas used are given in chapter six. It is shown how to obtain explicit formulas for the homogenized material property tensors for locally layered materials. In addition the sensitivity analysis for the update of the design variables is carried out.

In chapter seven the numerical methods used to solve the problems in the chapters before are discussed. It is shown how to use the finite element method to solve the occurring partial differential equations and iterative methods for the solution of the resulting systems of linear equations.

We conclude by noting that the results stated in chapter 3 and 4 have appeared in the literature, see [20], [21] and [22].
2. Linear Elasticity

In this chapter we give a basic overview of linear elasticity theory. After stating the constitutive law it is shown how the three dimensional equations lead by simplification to the cases of plane strain, plane stress and torsional rigidity. In the following chapters optimal design problems based on these cases are solved. Often in engineering the elastic behavior of a material is characterized by quantities called Young’s modulus and Poisson’s ratio whereas in mathematical modeling and computation shear and bulk modulus are used. We shortly explain the meaning of these properties and give the relations between them.

2.1 Three Dimensional Problem

Stress measures the internal distribution of force per unit area within a body as an reaction to the loads applied to it. Strain is an expression of deformation caused by the action of stress in a body. The kinematic or strain-displacement equations describe how the strains \( \epsilon \) within a loaded body relate to the body’s displacements \( u = (u_1, u_2, u_3)^T \)

\[
\epsilon = \begin{pmatrix}
\frac{\partial u_1}{\partial x_1} & \frac{1}{2} \left( \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) & \frac{1}{2} \left( \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1} \right) \\
\frac{1}{2} \left( \frac{\partial u_2}{\partial x_1} + \frac{\partial u_1}{\partial x_2} \right) & \frac{\partial u_2}{\partial x_2} & \frac{1}{2} \left( \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2} \right) \\
\frac{1}{2} \left( \frac{\partial u_3}{\partial x_1} + \frac{\partial u_1}{\partial x_3} \right) & \frac{1}{2} \left( \frac{\partial u_3}{\partial x_2} + \frac{\partial u_2}{\partial x_3} \right) & \frac{\partial u_3}{\partial x_3}
\end{pmatrix}.
\] (2.1)

For small deformations it will be assumed that the stress \( \sigma \) is directly proportional to the strain \( \epsilon \) in a linear elastic material. This is known as Hooke’s law relating the local stress to the local strain and is given by

\[
\sigma_{ij} = C_{ijkl} \epsilon_{kl}
\] (2.2)

where \( i, j, k, l = 1, \ldots, 3 \). The fourth order tensor \( C \) is called the stiffness or elastic tensor. For a general anisotropic material, the 81 elements of the stiffness tensor are all independent. Fortunately, there is no actual material which has 81 independent elastic parameters. In the absence of distributed couples, it follows from the equilibrium of moments of an elastic particle that the stress tensor is symmetric. Because of the definition of strains, it also follows that \( \epsilon \) is symmetric. Therefore the number of independent equations reduces from nine to six. As a consequence of the symmetries of \( \sigma \) and \( \epsilon \) we have that

\[
C_{ijkm} = C_{jikm} \quad \text{and} \quad C_{ijkm} = C_{ijmk}
\] (2.3)

and there are only 36 independent parameters left. The constitutive equation (2.2) can be rewritten in a compact form as

\[
\sigma_i = C_{ij} \epsilon_j, \quad i, j = 1, \ldots, 6
\] (2.4)

where the contracted stresses \( \sigma_i \) and strains \( \epsilon_j \) are defined as

\[
\begin{align*}
\sigma_1 &= \sigma_{11} & \sigma_2 &= \sigma_{22} & \sigma_3 &= \sigma_{33} & \sigma_4 &= \sigma_{12} & \sigma_5 &= \sigma_{13} & \sigma_6 &= \sigma_{23} \\
\epsilon_1 &= \epsilon_{11} & \epsilon_2 &= \epsilon_{22} & \epsilon_3 &= \epsilon_{33} & \epsilon_4 &= \epsilon_{12} & \epsilon_5 &= \epsilon_{13} & \epsilon_6 &= \epsilon_{23}.
\end{align*}
\] (2.5)

In the absence of residual stresses it follows that

\[
C_{ij} = C_{ji}
\] (2.6)
and the number of elastic constants reduces from 36 to 21. This is the most general case when the
material is anisotropic. Then the stress-strain relation (2.2) can be written in the form
\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{12} \\
\sigma_{13} \\
\sigma_{23}
\end{pmatrix} = \begin{pmatrix}
C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\
C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\
C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\
C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66}
\end{pmatrix} \begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{33} \\
\epsilon_{12} \\
\epsilon_{13} \\
\epsilon_{23}
\end{pmatrix}.
\] (2.7)

For isotropic materials the constants are reduced to 2. These moduli \(\lambda\) and \(\mu\) are known as the first and second Lamé constant. The system (2.7) can then be written as
\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{12} \\
\sigma_{13} \\
\sigma_{23}
\end{pmatrix} = \begin{pmatrix}
2\mu + \lambda & \lambda & \lambda & 0 & 0 & 0 \\
\lambda & 2\mu + \lambda & \lambda & 0 & 0 & 0 \\
\lambda & \lambda & 2\mu + \lambda & 0 & 0 & 0 \\
0 & 0 & 0 & 2\mu & 0 & 0 \\
0 & 0 & 0 & 0 & 2\mu & 0 \\
0 & 0 & 0 & 0 & 0 & 2\mu
\end{pmatrix} \begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{33} \\
\epsilon_{12} \\
\epsilon_{13} \\
\epsilon_{23}
\end{pmatrix}.
\] (2.8)

or, in indicial form,
\[
\sigma_{ij} = 2\mu\epsilon_{ij} + \lambda\delta_{ij}\epsilon_{kk}.
\] (2.9)

The terms \(\sigma_{11}, \sigma_{22}\) and \(\sigma_{33}\) are called normal stresses and the terms \(\sigma_{12}, \sigma_{13}\) and \(\sigma_{23}\) are called shear stresses. Normal stresses lead to a change in volume whereas shear stresses lead only to a change in shape.

It is common to use engineering material constants that are related to measurements from elementary mechanical tests instead of the Lamé constants. They describe the resistance of the material against certain deformations. In the following we provide a short overview of those quantities for isotropic materials.

**Poisson’s ratio** \(\nu\) is the ratio of transverse contraction to longitudinal extension in the direction of stretching force. Tensile deformation is considered positive and compressive deformation is considered negative. The Poisson’s ratio for elastic materials lies between \(-1 < \nu < 0.5\). For most materials \(\nu \approx 0.3\), cork is close to 0.0, and rubber almost 0.5.

**Young’s modulus** \(E\) [Pa], also known as the modulus of elasticity, is a measure of the stiffness of a material. It is defined as the ratio of stress to strain on the loading plane along the loading direction. For rubber \(E \approx 0.1\) GPa, for steel 200 GPa, and for diamond 1100 GPa.

The **shear modulus** \(G\) [Pa], the modulus of rigidity, is defined as the ratio of shear stress to shear strain. It can be determined by twisting tests. The shear modulus is equal to the second Lamé constant and also often called \(\mu\). In what follows we also use this notation for the shear modulus. For plywood \(\mu = 0.6\) GPa, for glass \(\mu = 18\) GPa, and for steel \(\mu = 79\) GPa.

The **bulk modulus** \(\kappa\) [Pa] measures the response in pressure due to a change in relative volume, essentially measuring the material’s resistance to uniform compression. It is the inverse of the compressibility
\[
\kappa = -V \frac{\partial P}{\partial V},
\] (2.10)
where \(P\) is the pressure and \(V\) is the volume. For air \(\kappa = 0.00014\) GPa, for water 2.2 GPa, and for steel 160 GPa.
For elastically anisotropic materials the elastic properties depend on the direction of the applied force. For fiber reinforced material for instance the values of $E$ in the direction of the fibers are higher than in the other directions and also the values of $\nu$ and $\mu$ are higher in the planes along the fiber than in the one across the fiber.

For future reference we note that the stiffness tensor can be written in terms of projection tensors

$$C = 3\kappa \Lambda_h + 2\mu \Lambda_s$$ (2.11)

where

$$(\Lambda_h)_{ijkl} = \frac{1}{3} \delta_{ij} \delta_{kl}$$ (2.12)

$$(\Lambda_s)_{ijkl} = \frac{1}{3} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) - \frac{1}{3} \delta_{ij} \delta_{kl}.$$ (2.13)

The tensor $\Lambda_h$ projects onto hydrostatic fields and the tensor $\Lambda_s$ projects onto shear fields. Combining (2.11) and (2.12)-(2.13) we obtain for (2.2)

$$\sigma = 2\mu (\epsilon - \frac{1}{3} \text{tr} I) + 3\kappa \frac{1}{3} \text{tr} I.$$ (2.14)

We can rewrite system (2.8) in terms of shear and bulk modulus

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{pmatrix} = \begin{pmatrix} \frac{4}{3} \mu + \kappa & \kappa - \frac{2}{3} \mu & \kappa - \frac{2}{3} \mu & 0 & 0 & 0 \\ \kappa - \frac{2}{3} \mu & \frac{4}{3} \mu + \kappa & \kappa - \frac{2}{3} \mu & 0 & 0 & 0 \\ \kappa - \frac{2}{3} \mu & \kappa - \frac{2}{3} \mu & \frac{4}{3} \mu + \kappa & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\mu \end{pmatrix} \begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{12} \\ \epsilon_{13} \\ \epsilon_{23} \end{pmatrix}.$$ (2.15)

Inverting relation (2.8) to express strains in terms of stresses we obtain

$$\epsilon_{ij} = S_{ijkl} \sigma_{kl}$$ (2.16)

$$\begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{12} \\ \epsilon_{13} \\ \epsilon_{23} \end{pmatrix} = \begin{pmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \frac{1}{2G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2G} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{pmatrix}.$$ (2.17)

where $S$ is the compliance tensor. This is more easily expressed using engineering constants and we write

$$\begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{12} \\ \epsilon_{13} \\ \epsilon_{23} \end{pmatrix} = \begin{pmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \frac{1}{2G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2G} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{pmatrix}.$$ (2.18)
Relation (2.8) in terms of engineering constants can be written as

\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{12} \\
\sigma_{13} \\
\sigma_{23}
\end{pmatrix} =
\begin{pmatrix}
\frac{E(1-\nu)}{(1+\nu)(1-2\nu)} & \frac{E\nu}{(1+\nu)(1-2\nu)} & \frac{E\nu}{(1+\nu)(1-2\nu)} & 0 & 0 & 0 \\
\frac{E\nu}{(1+\nu)(1-2\nu)} & \frac{E}{(1+\nu)} & \frac{E\nu}{(1+\nu)(1-2\nu)} & 0 & 0 & 0 \\
\frac{E\nu}{(1+\nu)(1-2\nu)} & \frac{E\nu}{(1+\nu)(1-2\nu)} & \frac{E}{(1+\nu)} & 0 & 0 & 0 \\
0 & 0 & 0 & 2G & 0 & 0 \\
0 & 0 & 0 & 0 & 2G & 0 \\
0 & 0 & 0 & 0 & 0 & 2G
\end{pmatrix}
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{33} \\
\epsilon_{12} \\
\epsilon_{13} \\
\epsilon_{23}
\end{pmatrix}. \tag{2.19}
\]

From the different expressions for stiffness and compliance tensor we obtain the relations between the quantities which are given in table 2.1.

<table>
<thead>
<tr>
<th>( \mu, \lambda )</th>
<th>( \mu, \kappa )</th>
<th>( E, \nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu )</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>( \lambda = \frac{3\kappa - 2\mu}{3} )</td>
<td>( \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} )</td>
</tr>
<tr>
<td>( \mu )</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( \kappa )</td>
<td>( \kappa = \frac{2\mu + 3\lambda}{3} )</td>
<td>( \kappa = \frac{E}{3(1-2\nu)} )</td>
</tr>
<tr>
<td>( E )</td>
<td>( E = \frac{\mu(2\mu + 3\lambda)}{\mu + \lambda} )</td>
<td>( E = \frac{9\kappa G}{3\kappa + G} )</td>
</tr>
<tr>
<td>( \nu )</td>
<td>( \nu = \frac{\lambda}{2(\mu + \lambda)} )</td>
<td>( \nu = \frac{3\kappa - 2G}{2(3\kappa + G)} )</td>
</tr>
</tbody>
</table>

So we obtain for a general elasticity problem: Find the displacements \( \mathbf{u} = (u_1, u_2, u_3)^T \) in a structure \( \Omega \) with boundary \( \Gamma \) for which

\[
-\text{div}\mathbf{\sigma}_{ij} = f_i \text{ on } \Omega \tag{2.20}
\]
\[
\sigma_{ij} = E_{ijkl}\epsilon_{ij} \tag{2.21}
\]
\[
\epsilon_{ij} = \frac{1}{2} (\partial_x u_j + \partial_x u_i) \tag{2.22}
\]
\[
\sigma_{ij} n_j = g_i \text{ on } \Gamma_1 \tag{2.23}
\]
\[
u_i = h_i \text{ on } \Gamma_2 \tag{2.24}
\]

and \( i, j = 1 \ldots 3 \). For more details about elasticity theory see for instance [33]. There are many situations where symmetry and loading allow to reduce the full three dimensional system of elasticity to a two dimensional system or a scalar equation. In the following we want to consider some of these cases.

### 2.2 Two Dimensional Problem

In two dimensions Hooke’s law can be formulated analogously to (2.14)

\[
\sigma = 2\mu(\epsilon - \frac{1}{2}\text{tr}I) + 2\kappa\frac{1}{2}\text{tr}I. \tag{2.25}
\]
or
\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{pmatrix} = \begin{pmatrix}
\mu + \kappa & \kappa - \mu & 0 \\
\kappa - \mu & \mu + \kappa & 0 \\
0 & 0 & 2\mu
\end{pmatrix} \begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{12}
\end{pmatrix}.
\]
(2.26)

There are two cases for isotropic two dimensional elasticity: plane strain and plane stress elasticity. To connect the moduli one must specify which case is treated. Plane strain elasticity is physically relevant in considering fiber-reinforced materials whereas plane stress elasticity is relevant in considering two phase composites in the form of thin sheets.

2.2.1 Plane Stress Problem
A plane stress problem is one in which the thickness is normally small compared to the profile. Examples are stretching or shearing of thin slabs or brackets. For plane stress with the \( z \)-axis stress-free, we have
\[
\sigma_{13} = \sigma_{23} = \sigma_{33} = 0.
\]
(2.27)

We also assume that the remaining stresses do not vary with \( z \), but are only functions of \( x \) and \( y \). Plugging in (2.27) in (2.18) we obtain
\[
\begin{align*}
\epsilon_{11} &= \frac{1}{E} (\sigma_{11} - \nu \sigma_{22}) \\
\epsilon_{22} &= \frac{1}{E} (-\nu \sigma_{11} + \sigma_{22}) \\
\epsilon_{33} &= -\nu E (\sigma_{11} + \sigma_{22}) \\
\epsilon_{12} &= \frac{1}{2\mu} \\
\epsilon_{13} = \epsilon_{23} &= 0.
\end{align*}
\]
(2.28-2.32)

From (2.30) we obtain a nonzero strain in the \( z \) direction indicating that a state of plane stress does not imply a corresponding state of plane strain. By writing (2.28), (2.29), and (2.31) together, relation (2.18) simplifies to
\[
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{12}
\end{pmatrix} = \begin{pmatrix}
\frac{1}{E} & -\frac{\nu}{E} & 0 \\
-\frac{\nu}{E} & \frac{1}{E} & 0 \\
0 & 0 & \frac{1}{2G}
\end{pmatrix} \begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{pmatrix}.
\]
(2.33)

Expressing stresses in terms of strains we have
\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{pmatrix} = \begin{pmatrix}
\frac{E}{1-\nu^2} & \frac{\nu E}{1-\nu^2} & 0 \\
\frac{\nu E}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 \\
0 & 0 & 2G
\end{pmatrix} \begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{12}
\end{pmatrix} = \begin{pmatrix}
2\mu + \lambda & \lambda & 0 \\
\lambda & 2\mu + \lambda & 0 \\
0 & 0 & 2\mu
\end{pmatrix} \begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{12}
\end{pmatrix}.
\]
(2.34)

Comparing equations (2.34) and (2.26) we obtain the relations between the Lamé constants and engineering constants in the plane stress case (table 2.2).

2.2.2 Plane Strain Problem
A plane strain problem is one in which the thickness is normally very large compared to the cross section. Examples are forces on cross sections of shafts. For plane strain with the \( z \)-axis strain-free, we have
\[
\epsilon_{13} = \epsilon_{23} = \epsilon_{33} = 0.
\]
(2.35)
TABLE 2.2. Relations between the elastic moduli for plane stress elasticity.

<table>
<thead>
<tr>
<th></th>
<th>$\mu$, $\lambda$</th>
<th>$\mu$, $\kappa$</th>
<th>$E$, $\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
<td>-</td>
<td>-</td>
<td>$\mu = \frac{E}{2(1 + \nu)}$</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>$\lambda = \kappa - \mu$</td>
<td>$\lambda = \frac{E}{\nu E(1 + \nu)(1 - \nu)}$</td>
<td></td>
</tr>
<tr>
<td>$\mu$</td>
<td>-</td>
<td>$\kappa = \mu + \lambda$</td>
<td>$\mu = \frac{E}{2(1 + \nu)}$</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>$\kappa = \mu + \lambda$</td>
<td>-</td>
<td>$\kappa = \frac{E}{2(1 - \nu)}$</td>
</tr>
<tr>
<td>$E$</td>
<td>$E = \frac{4\mu(\mu + \lambda)}{2\mu + \lambda}$</td>
<td>$E = \frac{4\kappa\mu}{\kappa + \mu}$</td>
<td>-</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$\nu = \frac{\lambda}{2\mu + \lambda}$</td>
<td>$\nu = \frac{\kappa - \mu}{\kappa + \mu}$</td>
<td>-</td>
</tr>
</tbody>
</table>

which implies that the cross section will remain plane. All tractions and body forces are functions of $x$ and $y$ only. Using (2.35) we obtain for (2.19)

$$
\sigma_{11} = \frac{E}{(1 + \nu)(1 - 2\nu)}(1 - \nu)\epsilon_{11} + \nu\epsilon_{22}
$$

(2.36)

$$
\sigma_{22} = \frac{E}{(1 + \nu)(1 - 2\nu)}(\nu\epsilon_{11} + (1 - \nu)\epsilon_{22})
$$

(2.37)

$$
\sigma_{33} = \frac{E\nu}{(1 + \nu)(1 - 2\nu)}(\epsilon_{11} + \epsilon_{22})
$$

(2.38)

$$
\sigma_{12} = 2\mu
$$

(2.39)

$$
\sigma_{13} = \sigma_{23} = 0.
$$

(2.40)

Similar to the plane stress problem we obtain a nonzero stress in the $z$ direction. Writing (2.36),(2.37), and (2.39) together, relation (2.19) simplifies to

$$
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{pmatrix} =
\begin{pmatrix}
\frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)} & \frac{E\nu}{(1 + \nu)(1 - 2\nu)} & 0 \\
\frac{E\nu}{(1 + \nu)(1 - 2\nu)} & \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)} & 0 \\
0 & 0 & 2\mu
\end{pmatrix}
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{12}
\end{pmatrix}.
$$

(2.41)

For plane strain elasticity the relations between the elastic moduli are given in table 2.3.

2.2.3 Torsional Rigidity and St. Venant’s Semi Inverse Method

We consider a shaft which is subjected to a twisting moment at the free end and restrained against both displacement and torsion at the other end. The solution of this torsion problem is due to St. Venant. The following assumptions are made:

1. The shaft is lying along the $x_3$ axis and fixed at $x_3 = 0$ and twisted at $x_3 = h$.
2. The rate of twist $\theta$ is constant.
3. Each cross section of the shaft rotates as a rigid body.
### Table 2.3: Relations between the elastic moduli for plane strain elasticity.

<table>
<thead>
<tr>
<th></th>
<th>$\mu$, $\lambda$</th>
<th>$\mu$, $\kappa$</th>
<th>$E$, $\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
<td>-</td>
<td>-</td>
<td>$\mu = \frac{E}{2(1+\nu)}$</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>-</td>
<td>$\lambda = \kappa - \mu$</td>
<td>$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>-</td>
<td>-</td>
<td>$\mu = \frac{E}{2(1+\nu)}$</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>$\kappa = \mu + \lambda$</td>
<td>-</td>
<td>$\kappa = \frac{E}{2(1+\nu)}$</td>
</tr>
<tr>
<td>$E$</td>
<td>$E = \frac{2(2\mu+\lambda+2)}{2\mu+\lambda}$</td>
<td>$E = \frac{\mu(3\kappa - \mu)}{\kappa}$</td>
<td>-</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$\nu = \frac{\lambda}{2\mu + 2}$</td>
<td>$\nu = \frac{\kappa - \mu}{2\kappa}$</td>
<td>-</td>
</tr>
</tbody>
</table>

4. Cross sections are free to deform extensionally in the $x_3$ direction but in the same way for all the cross sections.

The last assumption is the application of St. Venant’s semi inverse method to torsion problems.

Using the general elasticity problem (2.20)-(2.24) we obtain for the boundary conditions at $x_3 = 0$

$$u_1 = u_2 = u_3 = 0 \quad (2.42)$$

and at $x_3 = h$

$$u_1 = -\theta x_2 \quad (2.43)$$
$$u_2 = \theta x_1 \quad (2.44)$$

For $0 < x_3 < h$ we assume following St. Venant

$$u_1 = -\theta x_3 x_2 \quad (2.45)$$
$$u_2 = \theta x_3 x_1 \quad (2.46)$$
$$u_3 = \theta w(x_1, x_2). \quad (2.47)$$

Next we substitute this ansatz in the equations of elasticity (2.20)-(2.24) to obtain an equation for $w$. As a result we get for the strains

$$\epsilon_{11} = \epsilon_{22} = \epsilon_{33} = \epsilon_{12} = 0 \quad (2.48)$$
$$\epsilon_{13} = -\frac{\theta}{2}(x_2 + \partial x_1 w) \quad (2.49)$$
$$\epsilon_{23} = -\frac{\theta}{2}(x_1 + \partial x_2 w) \quad (2.50)$$

and for the stresses using (2.19)

$$\sigma_{11} = \sigma_{22} = \sigma_{33} = \sigma_{12} = 0 \quad (2.51)$$
$$\sigma_{13} = \theta G(\partial x_1 w - x_2) \quad (2.52)$$
$$\sigma_{23} = \theta G(\partial x_2 w + x_1). \quad (2.53)$$
Equation (2.20) becomes then
\[
\partial_{x_1}(\theta G(\partial_{x_1}w - x_2)) + \partial_{x_2}(\theta G(\partial_{x_2}w - x_1)) = 0 \quad (2.54)
\]

or
\[
div(G(\nabla w + v) = 0 \quad (2.55)
\]

and \(G = G(x_1, x_2)\). On the outside of the shaft we have
\[
G(\nabla w + v) = 0 \text{ on } \partial \Omega \quad (2.56)
\]

Introduce \(\phi\) the harmonic conjugate to \(w\) which is associated with a counterclockwise rotation and fulfills
\[
\begin{align*}
\partial_{x_1}\phi &= -\partial_{x_2}w \quad (2.57) \\
\partial_{x_2}\phi &= \partial_{x_1}w. \quad (2.58)
\end{align*}
\]

The function is defined uniquely up to an additive constant. The stress potential \(\Phi\) is defined as
\[
\Phi = G(\phi - \frac{1}{2}(x_1^2 + x_2^2)). \quad (2.59)
\]

We compute that
\[
\nabla \Phi = G(\nabla \phi - x) = RG(\nabla w + v) \quad (2.60)
\]

and obtain from this
\[
-div(2G^{-1}\nabla \phi) = 1 \quad (2.61)
\]

and \(\phi = 0\) on \(\partial \Omega\). The total torsional moment \(M\) of a cross section \(A\) is defined as
\[
M = \int_A F \times rdA = \int_A (x_1\sigma_{23} - x_2\sigma_{13})dx_1 dx_2 = \theta T \quad (2.62)
\]

where \(T\) is the torsional rigidity. \(T\) is a useful parameter for comparing the relative torsional stiffness of various cross sections. For a fixed twist \(\theta\) we have for the torsional rigidity
\[
T = \int_A (x_1\sigma_{23} - x_2\sigma_{13})dx_1 dx_2 \quad (2.63)
\]
\[
= \int_A \nabla \phi \cdot x dx_1 dx_2 \quad (2.64)
\]
\[
= 2 \int_A \phi dx_1 dx_2. \quad (2.65)
\]

In the following chapters is shown how to maximize the torsional rigidity for given cross sections and microstructure.
3. Fiber Reinforced Shaft

In this chapter we consider the problem of reinforcing a long shaft with constant cross section subject to torsion loading. The microstructure within the shaft consists of long reinforcement fibers of constant cross section with isotropic shear modulus $G_f$ embedded in a more compliant material with shear modulus $G_m$. The shaft together with the fibers are right cylinders with generators along the $x_3$ axis. The cross section of the reinforced shaft is specified by the region $\Omega$ in the $x_1 - x_2$ plane. In the neighborhood of any point $\mathbf{x} = (x_1, x_2)$ the local microgeometry is given by a periodic geometry with period cell filled with the Hashin Shtrikman coated cylinder assemblage [13], see figure 3.1.

![Cross section of a shaft filled with a graded locally periodic Hashin Shtrikman coated cylinder assemblage. The change in the local fiber area fraction across the structure is illustrated.](image)

3.1 Homogenized Design Formulation and Identification of Optimal Graded Fiber Microgeometries

The inverse homogenization design method is a top down design approach. First a well posed homogenized design problem is developed. This design problem is given in terms of design variables that reflect the local microgeometry inside the composite. For the problem treated here the design variable for the homogenized design problem is given by the local density of fibers $\theta_f(\mathbf{x})$ for points $\mathbf{x}$ in the shaft cross section. The homogenized design problem is then solved to obtain an optimal density function. With the optimal density in hand we use it to recover an explicit graded fiber design that has structural properties close to that of the optimal homogenized design and satisfies prescribed pointwise stress constraints. The homogenized design problem is described in the first subsection. The explicit link between homogenized
designs and graded fiber reinforced designs that satisfy pointwise stress constraints is provided in the second subsection.

### 3.1.1 Homogenized Design Problem

The design variable for the homogenized design problem is given by the density function \( \theta_f(x) \). This function is interpreted as providing the local area fraction of the fiber phase in a homogenized design. The resource constraint on the fiber phase is given by

\[
\int_\Omega \theta_f(x) \, dx_1 \, dx_2 \leq \Theta \times (\text{Area of } \Omega),
\]

where \( 0 < \Theta < 1 \). At each point the local area fraction satisfies the box constraint given by

\[
0 < \theta_{f}^{\text{min}} \leq \theta_f \leq \theta_{f}^{\text{max}} < 1.
\]

Here the upper and lower bounds given in (3.2) correspond to the entire design domain being filled with composite material. In this treatment the local fiber area fraction \( \theta_f \) changes continuously with position according to the condition

\[
|\theta_f(x) - \theta_f(x + h)| \leq K|h|.
\]

Here the constant \( K \) is prescribed by the designer. The universe of admissible designs given by all local area fractions \( \theta_f \) satisfying the resource constraint, box constraints, and (3.3) is denoted by \( D_{\Theta} \).

The compliance in shear for the matrix and fiber are given by \( S_m = (2G_m)^{-1} \) and \( S_f = (2G_f)^{-1} \) respectively. Here the matrix is more compliant and \( S_m > S_f \). The effective shear compliance \( S^E(\theta_f) \) for the Hashin Shtrikman coated sphere assemblage made from stiff fibers with area fraction \( \theta_f \) is given by [13]

\[
S^E(\theta_f(x)) = S_m \left( \frac{S_m + S_f + \theta_f(x)(S_f - S_m)}{S_m + S_f + \theta_f(x)(S_f + S_m)} \right).
\]

The macroscopic stress potential \( \phi^H \) vanishes on the boundary of the shaft cross section and satisfies

\[
-\text{div} \left( S^E(\theta_f) \nabla \phi^H \right) = 1
\]

inside the cross section. The torsional rigidity for the homogenized shaft cross section made from a homogenized material with compliance \( S^E(\theta_f) \) is given by

\[
\mathcal{R}(\theta_f) = 2 \int_\Omega \phi^H \, dx_1 \, dx_2.
\]
macroscopic stress is given by \( \sigma(x, y) = R[\nabla_y (w(x, y)) + \nabla \phi^H(x)] \), where for each \( x \) in the shaft cross section \( \Omega \) the \( Q \) periodic fluctuating stress potential \( w(x, y) \) solves the microscopic equilibrium equation

\[
- \text{div}_y \left( S(\theta_f(x), y)(\nabla_y (w(x, y)) + \nabla \phi^H(x)) \right) = 0, \quad y \in Q. \tag{3.7}
\]

Here the \( x \) coordinate appears as a parameter. The relevant interaction is described by the macrostress modulation function \( f(\theta_f, \sigma^H) \) given by

\[
f(\theta_f(x), \sigma^H(x)) = \sup_{y \in Q} \{|\sigma(x, y)|^2\}. \tag{3.8}
\]

Physically the macrostress modulation provides an upper envelope on the oscillating pointwise local stress in the composite [15], [16].

The macrostress modulation is calculated explicitly for the Hashin Shtrikman coated cylinder assemblage in [16]. We define the amplification factor

\[
A(\theta_f) = \left( \frac{2S_m}{S_m + S_f + \theta_f(S_m - S_f)} \right)^2 \tag{3.9}
\]

and set

\[
f(\theta_f, v) = A(\theta_f)|v|^2 \text{ if } \theta_f > 0 \text{ and } f(\theta_f, v) = |v|^2, \text{ if } \theta_f = 0 \tag{3.10}
\]

for every vector \( v \). Here \( A(\theta_f) \geq 1 \) and \( A(0) = (2S_m/(S_m + S_f))^2 > 1 \). In the context of torsional rigidity the macrostress modulation is written in terms of the homogenized stress potential and is given by

\[
f(\theta_f(x), \nabla \phi^H(x)). \tag{3.11}
\]

It is pointed out that the Hashin Shtrikman coated cylinder assemblage gives the smallest amplification factor \( A(\theta_f) \) among all locally periodic fiber microstructures with isotropic effective shear compliance [19].

We choose a subset \( S \) of the shaft cross section that lies a finite distance away from the boundary. On this set the prescribed multiscale stress criterion is given by

\[
f(\theta_f(x), \nabla \phi^H(x)) \leq T^2. \tag{3.12}
\]

In this treatment domains with reentrant corners are considered so there will be a stress singularity at the corner. Therefore the choice of \( T > 0 \) depends on the distance between \( S \) and the reentrant corner. It is clear that the multiscale stress criterion may not be satisfied by any homogenized design if \( T \) is chosen too small.

The homogenized design problem is given by

\[
HP = \left\{ \inf \{ R(\theta_f) \} ; \text{ subject to: } \begin{cases} \theta_f \text{ in } D_\Theta, \\ f(\theta_f(x), \nabla \phi^H(x)) \leq T^2, \text{ for } x \in S \end{cases} \right\}. \tag{3.13}
\]

The homogenized design problem \( HP \) is well posed and there is an optimal design \( \hat{\theta}_f \) provided \( T \) is chosen large enough so that the constraint set of (3.13) contains at least one design, see [17]. We mention in closing that the constraint (3.3) provides an upper bound on the spatial variation of the homogenized designs. This constraint provides the compactness necessary for a well posed design problem [17]. We conclude by noting that the theoretical basis for the approach given here has been established for three dimensional structural design using multiphase locally periodic composites in the presence of pointwise stress constraints see ([17], Theorems 5.1 and 5.2). For locally layered microstructures the corresponding theory is presented in [20].
3.1.2 Identification of Graded Fiber Design from the Homogenized Design

In this subsection it is shown how to use the optimal design $\hat{\theta}_f$ of $\hat{HP}$ to identify a graded fiber design satisfying the requirements (I) and (II). The building block for the microstructure is the unit cell filled with a Hashin Shtrikman coated cylinder assemblage [13]. The coated cylinder assemblage is constructed as follows. A space filling configuration of disks of different sizes ranging down to the infinitesimal is placed inside the unit period cell given by the unit square $Q$. Each disk is then partitioned into an annulus called the coating and a concentric disk which is a fiber cross section. The union of these “coated disks” make up the coated cylinder assemblage. The area fraction of the fiber phase is the same for all coated disks in the assemblage and is given by $\theta_f$. The union of the coatings comprises the matrix phase. The area fraction of the fiber phase for the coated cylinder assemblage inside the unit square is easily seen to be $\theta_f$. The unit square filled with the coated cylinder assemblage is illustrated in figure 3.1. A microstructure is obtained by rescaling the unit cell by the factor $\varepsilon$ so that it becomes the period cell for an $\varepsilon$ periodic composite.

In order to describe the graded fiber composite one partitions the shaft cross section $\Omega$ into the $N$ subdomains $\omega^k$, $k = 1, \ldots, N$ and $\Omega = \bigcup_n^N \omega^k$. The maximum diameter of the subdomains in the partition is denoted by $\tau_N$. The partition is denoted by $P_{\tau_N}$. A graded fiber composite is constructed by placing an $\varepsilon$ periodic Hashin Shtrikman coated cylinder geometry inside each subdomain $\omega^k$. The area fraction of fibers in each subdomain is given by the constant $\theta_f$ and these constants can change between subdomains. For future reference this type of locally periodic microstructure will be called a $(\tau_N, \varepsilon)$-graded Hashin Shtrikman fiber microstructure. The local piecewise constant shear compliance for the $(\tau_N, \varepsilon)$-graded Hashin Shtrikman coated fiber microstructure is denoted by $S_{\varepsilon,N}$. The stress potential for this microstructure is denoted by $\phi_{\varepsilon,N}$ and vanishes on the boundary of the cross section. Furthermore the stress potential satisfies the equilibrium equation

$$-\text{div} \left( S_{\varepsilon,N} \nabla \phi_{\varepsilon,N} \right) = 1. \quad (3.14)$$

The torsional rigidity of the cross section is given by

$$R_{\varepsilon,N} = 2 \int_\Omega \phi_{\varepsilon,N} \, dx_1 \, dx_2. \quad (3.15)$$

The nonzero components of the in plane stress are denoted by the vector $\sigma_{\varepsilon,N} = (\sigma_{13}^{\varepsilon,N}, \sigma_{23}^{\varepsilon,N})$ and are related to the gradient of the stress potential according to

$$\sigma_{\varepsilon,N} = R \nabla \phi_{\varepsilon,N}. \quad (3.16)$$

Here $R$ is the matrix corresponding to a counterclockwise rotation of $\pi/2$ and $|\sigma_{\varepsilon,N}| = |\nabla \phi_{\varepsilon,N}|$.

Given any partition $P_{\tau_N}$ the partition $P_{\tau_N}$ is said to be a refinement of it, if $\tau_N < \tau_N$ and if each subdomain belonging to $P_{\tau_N}$ is a subset of a subdomain in $P_{\tau_N}$. Next for any given partition $P_{\tau_N}$ we introduce a nested sequence of refinements $\{P_{\tau_N}^{N+1}\}_{N=1}^\infty$ such that $P_{\tau_N}^{N+1} = P_{\tau_N}$ and $P_{\tau_N}^{N+1}$ is a refinement of $P_{\tau_N}^{N+1}$ with $\lim_{\ell \to \infty} \tau_{N+1}^{N+1} = 0$. Here we assume $\varepsilon < \tau_{N+1}$ and we will consider the sequence of $(\tau_{N+1}, \varepsilon)$-graded Hashin Shtrikman fiber microstructures with associated stress potentials $\phi_{\varepsilon,N}(x)$.

The identification of a graded fiber composite satisfying the pointwise stress constraints is given in the following Proposition.

**Proposition 3.1. Identification of graded microstructure.**

Consider a homogenized design specified by $\theta_f$ in $D_\Theta$ such that the multiscale stress criterion (3.12) holds on the subset $S$ of the shaft cross section. Consider also any partition $P_{\tau_N}$ of the design domain...
Then for any given \( t > T \) and small number \( \delta > 0 \), there is a refinement \( \mathcal{P}^{N_t} \) of the partition and an associated \((\tau_{N_t}, \varepsilon)\)-graded Hashin Shtrikman fiber microstructure for which the part of \( S \) over which

\[
|\nabla \phi^{\varepsilon, N_t}(x)| \leq t
\]

is violated has measure (area) less than \( \delta \) and

\[
|\mathcal{R}^{\varepsilon, N_t} - \mathcal{R}(\theta_f)| < \delta,
\]

and

\[
\sum_{k=1}^{N_t} \omega_k \theta_f^k \leq \Theta \times \text{(Area of } \Omega) + \delta. \tag{3.19}
\]

Here \( |\omega_k| \) denotes the area of \( \omega_k \). Moreover the area fractions \( \theta_f^k \) are determined from \( \theta_f \) through the averages given by

\[
\theta_f^k = \frac{1}{|\omega_k|} \times \int_{\omega_k} \theta_f(x) dx_1 dx_2. \tag{3.20}
\]

This Proposition is established in [17]. The homogenized design formulation together with Proposition 3.1 provide an inverse homogenization method for identifying microstructures that satisfy pointwise stress constraints while delivering a torsional rigidity close to that given by the optimal design \( \hat{\theta}_f \) for the homogenized design problem.

### 3.2 Gradient Algorithm for the Homogenized Design Problem

In the computational examples we enforce the stress constraint by adding a penalty term to the torsional rigidity and minimize

\[
L(\theta_f) = -\mathcal{R}(\theta_f) + l \int_{\Omega} (f(\theta_f, \nabla \phi^H))^p dx_1 dx_2, \tag{3.21}
\]

over all \( \theta_f \) in \( D_\Theta \) where \( l > 0 \) and \( \phi^H \) satisfies

\[
-\text{div} \left( S^E(\theta_f) \nabla \phi^H \right) = 1 \tag{3.22}
\]

and vanishes at the boundary. The computational examples provided here will be carried out for a domain with reentrant corners of interior angle \( 3\pi/2 \). In view of the strength of the associated singularity at the reentrant corners the power “\( p \)” appearing in the penalty term is chosen to be less than 3. This minimization problem is well posed and one can find a minimizing density \( \hat{\theta}_f(x) \) see [17].

Given the minimizing density and associated stress potential \( \hat{\phi}^H \) one considers sets of the form

\[
A_T = \{ x \in \Omega : f(\hat{\theta}_f(x), \nabla \hat{\phi}^H(x)) \leq T^2 \}. \tag{3.23}
\]

For fixed choices of \( \delta > 0 \) and \( t > T \) proposition 3.1 can be used to recover a \((\tau_N, \varepsilon)\)-graded Hashin Shtrikman fiber microstructure for which the part of \( A_T \) over which the stress constraint

\[
|\nabla \phi^{\varepsilon, N}(x)| \leq t \tag{3.24}
\]

is violated has measure less than \( \delta \),

\[
|\mathcal{R}^{\varepsilon, N} - \mathcal{R}(\hat{\theta}_f)| < \delta, \tag{3.25}
\]
and

$$\sum_{k=1}^{N} |\omega^k| \theta_j^k \leq \Theta \times (\text{Area of } \Omega) + \delta. \quad (3.26)$$

Here the area fractions $\hat{\theta}_j^k$ are given by

$$\hat{\theta}_j^k = \frac{1}{|\omega^k|} \times \int_{\omega^k} \hat{\theta}_j(x) dx_1 dx_2. \quad (3.27)$$

To proceed numerically we compute the derivative of the objective function given by (3.21) with respect to the design variable $\theta_f$. The derivative will be used to develop a gradient minimization algorithm. The design domain is filled with composite and $0 \leq \theta_f^\text{min} \leq \theta_f \leq \theta_f^\text{max} < 1$ at each point in the design domain. For our computations we choose $\theta_f^\text{min} = 0.01$ and $\theta_f^\text{max} = 0.99$. For this choice the modulation function is differentiable with respect to the density and we develop a gradient method subject to the constraints.

The gradient of the objective is computed with the help of an adjoint field $\lambda$. Here $\lambda$ is the solution of

$$-\text{div} \left( S^E(\theta_f) \nabla \lambda \right) = 1 + l \text{div} \left( 2p(A(\theta_f) \nabla \phi^H \cdot \nabla \phi^H)^{p-1} A(\theta_f) \nabla \phi^H \right). \quad (3.28)$$

where $1 \leq p < 3$ and $\lambda = 0$ on the boundary. For $\eta << 1$ the change in the stress potential $\phi^H$ due to small local perturbations $\eta \theta_f$ in the area fraction, is written as $\tilde{\phi}$ and

$$-\text{div} \left( S^E(\theta_f) \nabla \tilde{\phi} \right) = \text{div} \left( (\partial_{\theta_f} S^E(\theta_f) \tilde{\theta}_f) \nabla \phi^H \right) \quad (3.29)$$

where $\tilde{\phi} = 0$ on the boundary. Applying standard arguments using (3.22), (3.28) and (3.29) one calculates to first order that

$$\Delta L = \eta \int_{\Omega} \partial_{\theta_f} L \tilde{\theta}_f dx_1 dx_2, \quad \text{where}$$

$$\partial_{\theta_f} L = \partial_{\theta_f} S^E(\theta_f) \nabla \lambda \cdot \nabla \phi^H + 2lp(A(\theta_f) \nabla \phi^H \cdot \nabla \phi^H)^{p-1} \partial_{\theta_f} A(\theta_f) \nabla \phi^H \cdot \nabla \phi^H. \quad (3.30)$$

The continuity constraints on $\theta_f(x)$ expressed by (3.3) are enforced by the way in which the design variable is initialized and updated. The local average of a scalar function $f$ over the disk of radius $R$ centered at $p$ is denoted by $< f >^R (p)$. For a given field $\theta_f$ satisfying the resource constraint (3.1) and box constraint $\theta_f^\text{min} \leq \theta_f \leq \theta_f^\text{max}$ the initial choice of design variable $\theta_f^0$ is given by

$$\theta_f^0 = (\theta_f)^R (x). \quad (3.31)$$

At the $n$th step we suppose that $\theta_f^n$ is given and we solve for $\phi^H$ and $\lambda$ using the system of equations (3.22) and (3.28). The design variable $\theta_f^n$ is updated according to

$$\theta_f^{n+1} = (\theta_f^n - \eta \partial_{\theta_f} L)^R (x) \quad (3.32)$$

were $\partial_{\theta_f} L$ is given by (3.30). If the right hand side of (3.32) lies out side the box constraint $\theta_f^\text{min} \leq \theta_f \leq \theta_f^\text{max}$ we update according to

$$\theta_f^{n+1} = \theta_f^\text{min}, \text{ if } (\theta_f^n - \eta \partial_{\theta_f} L)^R (x) < \theta_f^\text{min} \text{ and}$$

$$\theta_f^{n+1} = \theta_f^\text{max}, \text{ if } (\theta_f^n - \eta \partial_{\theta_f} L)^R (x) > \theta_f^\text{max}. \quad (3.33)$$
Because the updated functions are given by averages of bounded functions it is easily seen that they satisfy (3.3) for a non-negative constant $K$ independent of $x$. The use of local averaging in the update scheme is similar to the use of filters in topology optimization see [4] and [5].

For points near the boundary a difficulty arises when defining the averages. This is dealt with by extending $\theta_f$ to the slightly larger domain $\Omega_R = \{x \in \mathbb{R}^2; \text{dist}(x, \Omega) \leq R\}$. The particular form of extension is up to the designer. Possibilities include setting $\theta_f = \theta_f^{\text{max}}$ in $\Omega_R \setminus \Omega$ or reflection of $\theta_f$ across the boundary of $\Omega$ into $\Omega_R$. In the discretized problem used for the simulations we allow $\theta_f$ to take constant values inside each element and define $\langle \theta_f \rangle^R$ to be the average of $\theta_f$ taken over all neighboring elements.

### 3.3 Inverse Homogenization for the X-shaped Cross Section

The computational examples are carried out for an “X” shaped domain. All interior angles for the reentrant corners are fixed at $3\pi/2$ radians. The shear stiffness of the matrix is assigned the value $G_m = 1 \text{GPa}$ and the shear stiffness of the fiber phase is assigned the value $G_f = 2 \text{GPa}$. For these choices $S_m = 1/(2G_m) = 0.5$ and $S_f = 1/(2G_f) = 0.25$. All of the design optimizations are carried out with the matrix material occupying 70% of the shaft cross section. The local fiber area fraction $\theta_f$ is constrained to lie in the interval $0.01 \leq \theta_f \leq 0.99 < 1$.

In the first example we optimize for torsional rigidity only. The resulting optimal design is referred to as design 1. The color scale plot of the local area fraction of matrix material $\hat{\theta}_m = 1 - \theta_f$ is given in figure 3.4. Here the lightest blue regions corresponds to points where $\hat{\theta}_m = 0$. The red regions correspond to points where $\theta_m = 0.99$. As expected this design ignores the stress concentration at the reentrant corners and a zone of stiff material surrounds a more compliant inner core and lies adjacent to the reentrant corners. In the next example the torsional rigidity is optimized in the presence of an integral penalization $\int (f)^1$, i.e., $p = 1$ for the lagrangian in (3.21). The resulting design is referred to as design 2. The plot of $\hat{\theta}_m$ for this design is given in figure 3.5. For this case it is seen that there is a topology change in the design and the more compliant material now surrounds the stiffer material shielding it from the stress concentration at the reentrant corners. In the final example the torsional rigidity is optimized in the presence of a stronger integral penalization given by $\int (f)^2$, i.e., $p = 2$ for the lagrangian in (3.21). The resulting design is referred to as design 3. The plot of $\hat{\theta}_m$ for this design is given in figure 3.6. As in design 2 it is seen that the more compliant material shields the stiff material from the stress concentration at the reentrant corners. The associated torsional rigidities for each of these cases are listed in table 3.1. It is seen from the table that the torsional rigidity drops by 44% for the stress constrained designs.

The contour plot of the macrostress modulation function $f$ for design 1 is given in figure 3.7. Figures 3.8 and 3.9 give the contour plots for $f$ in designs 2 and 3 respectively. When comparing designs 1, 2 and 3 it is clear from figures 3.7, 3.8 and 3.9 that designs 2 and 3 provide a significant reduction in the size of the over stressed zone $f \geq 1$.

It is pointed out that proposition 3.1 provides a rigorous general method for constructing a $(\tau_N, \varepsilon)$-graded Hashin Shtrikman fiber microstructure from the data given in design 2. To fix ideas we choose a tolerance $\delta = 1/1000$ and $t = 1.001$. Then proposition 3.1 shows how to construct a $(\tau_N, \varepsilon)$-graded Hashin Shtrikman fiber microstructure with torsional rigidity $R^{\varepsilon,N}$ satisfying

$$|R^{\varepsilon,N} - 0.204| < 1/1000$$

(3.34)

and for which the magnitude of the in plane stress lies below 1.001 for all points in the region $f < 1$ of figure 3.8, with the possible exception of a subset of points of area less than 1/1000.
3.4 Inverse Homogenization for a Fiber Microgeometry with Variation on One Scale

The local fields inside the Hashin Shtrikman coated cylinder assemblage provide a good approximation to the local fields inside long fiber reinforced shafts even when the fiber radii \( r \) are constrained to lie within a preset range \( r_{\text{min}} \leq r \leq r_{\text{max}} \). This is illustrated in figures 3.2 and 3.3 where the maximum value of the local stress amplitude and effective properties are plotted as functions of area fraction for the Hashin Shtrikman assemblage and for a single centered fiber inside a square period cell. Motivated by this observation we consider a design problem for shafts reinforced with a periodic array of fibers with radii constrained to lie with in a prescribed interval. The inverse homogenization method is applied to identify a graded distribution of fiber radii that impart desirable stiffness properties while constraining the extent of highly stressed zones due to reentrant corners.

The periodic lattice considered here is generated by square period cells. The fiber configuration is given by a single fiber centered inside each period cell and the radii of each fiber is chosen independently of the others. For future reference let \( S_i \) denote the \( i^{th} \) period cell in the lattice. Two examples are carried out, the first is for a lattice spacing of 0.0666 and the second is for a lattice spacing of 0.133. For the first example \( r_{\text{min}} = 0.0333 \), \( r_{\text{max}} = 0.063 \) and for the second example \( r_{\text{min}} = 0.01665 \), \( r_{\text{max}} = 0.0315 \). The homogenized design problem (HP) is carried out for \( \theta_f^{\text{min}} = 0.2 \) and \( \theta_f^{\text{max}} = 0.7 \) and \( p = 1 \). These choices are consistent with the choices of lattice spacings and minimum and maximum radii for each of the discrete design problems. The density of matrix material \( \theta_m(x) \) is plotted in figure 3.10. This design is denoted as design 4. The torsional rigidity for design 4 is 0.204. The contour plot of the macrostress modulation function for this design is given in figure 3.13. We follow the prescription of proposition 3.1 and use the results of the homogenized problem to construct the discrete fiber designs as follows. For each square \( S_i \) in the lattice we compute the average of \( \theta_f(x) \) over that square and denote it by \( \langle \theta_f \rangle_i \). The radius of the fiber in \( S_i \) chosen so that the fiber occupies the area fraction of the square given by \( \langle \theta_f \rangle_i \). The resulting designs are displayed in figures 3.11 and 3.12. The resulting design for lattice spacing 0.0666 is denoted as design 4A and for lattice spacing 0.133 is denoted as design 4B. The torsional rigidities for designs 4A and 4B are given by 0.227 and 0.225 respectively. The level lines of the magnitude of the stress field in design 4B is plotted in figure 3.15 and the level lines of the magnitude of the stress field in design 4A is plotted in figure 3.14. It follows from figures 3.13, 3.14, and 3.15 that pointwise stress behavior in designs 4A and 4B are well predicted by the level curves of the macrostress modulation function for the optimal homogenized design.

<table>
<thead>
<tr>
<th>Design #</th>
<th>Stress Constraint</th>
<th>Matrix-Volume Fraction</th>
<th>Torsional Rigidity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>None</td>
<td>70%</td>
<td>0.368</td>
</tr>
<tr>
<td>2</td>
<td>( f(f)^1 )</td>
<td>70%</td>
<td>0.204</td>
</tr>
<tr>
<td>3</td>
<td>( f(f)^2 )</td>
<td>70%</td>
<td>0.204</td>
</tr>
</tbody>
</table>
FIGURE 3.2. Effective property as function of area fraction.

FIGURE 3.3. Maximum value of the local stress amplitude as function of area fraction.
FIGURE 3.4. Design 1. Color plot of the area fraction of matrix material inside the X-shaped shaft cross section optimized for torsional rigidity only. Light blue regions are made exclusively of stiff fiber-phase material. Red regions contain only 1% by area fraction of fiber phase material.

FIGURE 3.5. Design 2. Area fraction distribution of matrix material inside the X-shaped cross section optimized for torsional rigidity with $p = 1$ integral penalty on $f$. 

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FIGURE 3.6. Design 3. Area fraction distribution of matrix material inside the X-shaped cross section optimized for torsional rigidity with \( p = 2 \) integral penalty on \( f \).

FIGURE 3.7. Contour plot of \( f \) for design 1.

FIGURE 3.8. Contour plot of \( f \) for design 2.
FIGURE 3.9. Contour plot of $f$ for design 3.

FIGURE 3.10. Contour plot of $\theta_f$ for design 4.

FIGURE 3.11. Fiber reinforced design 4A.
FIGURE 3.12. Fiber reinforced design 4B.

FIGURE 3.13. Contour plot of $f$ for design 4 with $p = 1$ penalty.

FIGURE 3.14. Contour plot of the magnitude of pointwise stress for design 4A.
FIGURE 3.15. Contour plot of the magnitude of pointwise stress for design 4B.
4. Locally Layered Materials

In this chapter we consider like in chapter 3 the problem of reinforcing a long shaft with constant cross section subject to torsion loading. The microstructure within the shaft consists of long reinforcement fibers of constant cross section with isotropic shear modulus $G_f$ embedded in a more compliant material with shear modulus $G_m$. The characteristic length scale of the microgeometry is assumed to be small relative to the dimensions of the shaft cross section and is denoted by $\varepsilon$. In the neighborhood of any point $\mathbf{x} = (x_1, x_2)$ the local microgeometry is given by layers of stiff material interspersed with layers of compliant material. The thickness of the stiff and compliant layers are specified by $\varepsilon \theta_1$ and $\varepsilon \theta_2$ respectively, with $\theta_1 + \theta_2 = 1$. The layer normals are specified by the angle $\gamma$. The thickness of the layers and layering orientation is free to change across the cross section, see figure 4.1.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{Figure4.png}
\caption{Domain filled with a graded locally layered microstructure. The local layer orientations in the neighborhood of the points $\mathbf{x}$ and $\mathbf{x}'$ are displayed.}
\end{figure}

4.1 Inverse Homogenization Method

In this section we state the homogenized design problem and provide the explicit connection between the optimal homogenized design and a desirable locally layered microgeometry that satisfies pointwise stress constraints while delivering a torsional rigidity close to that of the optimal homogenized design.

The design variables for the homogenized design problem are given by the local relative layer thickness of material one $\theta_1$ and the layer angle $\gamma$. The relative layer thickness of material two is denoted by $\theta_2$ and $\theta_1 + \theta_2 = 1$. The associated vector of design variables is denoted by $\mathbf{B}$ and $\mathbf{B}(\mathbf{x}) = (\theta_1(\mathbf{x}), \gamma(\mathbf{x}))$. The resource constraint on the amount of stiff material that can be used to reinforce the shaft cross section is given by

$$\int_{\Omega} (1 - \theta_1(\mathbf{x})) \, dx_1 dx_2 \leq \Theta \times (\text{Area of } \Omega), \quad (4.1)$$

where $0 < \Theta < 1$. At each point the design vector satisfies the box constraints given by

$$0 < \theta_1^{\text{min}} \leq \theta_1 \leq \theta_1^{\text{max}} < 1 \text{ and } 0 \leq \gamma \leq 2\pi. \quad (4.2)$$

Here the constraints on the relative layer thickness $\theta_1$ correspond to microstructured material filling out the entire design domain. The local microgeometry specified by $\mathbf{B}$ changes continuously with position.
and

\[ |\theta_1(x) - \theta_1(x + h)| \leq K|h|^{\alpha}, \]
\[ |\gamma(x) - \gamma(x + h)| \leq K|h|^{\alpha}, \] (4.3)

for fixed constants \(K\) and \(\alpha\) such that \(0 < \alpha \leq 1\). The set of all design vectors \(B\) satisfying the resource constraint, box constraints, and (4.3) is denoted by \(D_{\Theta}\).

The compliance in shear for each material is given by \(S_1 = (2G_1)^{-1}\) and \(S_2 = (2G_2)^{-1}\). Here material one is assumed to be the more compliant material, i.e., \(S_1 > S_2\). The effective compliance tensor \(S^E(B)\) is given by

\[ S^E(B(x)) = R(\gamma(x))D(\theta_1(x))R^T(\gamma(x)), \] (4.4)

where \(R(\gamma)\) is the matrix associated with a counterclockwise rotation of \(\gamma\) radians and \(D(\theta_1)\) is the \(2 \times 2\) diagonal matrix given by

\[ D(\theta_1) = \begin{bmatrix} (\theta_1 S_1^{-1} + (1 - \theta_1) S_2^{-1})^{-1} & 0 \\ 0 & \theta_1 S_1 + (1 - \theta_1) S_2 \end{bmatrix}. \] (4.5)

The macroscopic stress potential \(\phi^H\) vanishes on the boundary of the cross section and satisfies

\[ -\text{div} \left( S^E(B) \nabla \phi^H \right) = 1 \] (4.6)

inside the cross section. The torsional rigidity for the homogenized shaft cross section made from a homogenized material with compliance \(S^E(B)\) is given by

\[ \mathcal{R}(B) = 2 \int_{\Omega} \phi^H \, dx_1 \, dx_2. \] (4.7)

The stress in the homogenized shaft is given by \(\sigma^H = R \nabla \phi^H\) where \(R\) is the rotation matrix associated with a counterclockwise rotation of \(\pi/2\) radians.

The macroscopic stress constraints associated with materials one and two are given in terms of the macrostress modulation functions introduced in [15]. We define the matrices

\[ Q_1(B(x)) = R(\gamma(x))(\Lambda_1(\theta_1(x)))^2 R^T(\gamma(x)) \]
\[ Q_2(B(x)) = R(\gamma(x))(\Lambda_2(\theta_1(x)))^2 R^T(\gamma(x)), \] (4.8)

where the \(2 \times 2\) matrices \(\Lambda_1(\theta_1)\) and \(\Lambda_2(\theta_1)\) are given by

\[ \Lambda_1(\theta_1) = \begin{bmatrix} 1 - \frac{(S_2 - S_1)(1 - \theta_1)}{\theta_1 S_1 + (1 - \theta_1) S_2} & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \Lambda_2(\theta_1) = \begin{bmatrix} 1 + \frac{(S_2 - S_1)\theta_1}{\theta_1 S_1 + (1 - \theta_1) S_2} & 0 \\ 0 & 1 \end{bmatrix}. \] (4.9)

The explicit formula for the macrostress modulations are given by

\[ f_1(B(x), v) = Q_1(B(x))v \cdot v \quad \text{if} \quad \theta_1(x) > 0 \quad \text{and} \quad f_1(B(x), v) = 0, \quad \text{if} \quad \theta_1 = 0 \] (4.11)
\[ f_2(B(x), v) = Q_2(B(x))v \cdot v \quad \text{if} \quad \theta_2(x) > 0 \quad \text{and} \quad f_2(B(x), v) = 0, \quad \text{if} \quad \theta_2 = 0 \] (4.12)

for every vector \(v\). We choose a subset \(S\) of the shaft cross section that lies a finite distance away from the boundary. On this set the prescribed macroscopic stress constraints are given by

\[ f_1(B(x), \nabla \phi^H(x)) \leq T^2 \] (4.13)
\[ f_2(B(x), \nabla \phi^H(x)) \leq T^2. \] (4.14)
In this treatment, domains with reentrant corners are considered and so there will be a stress singularity at the corner. Therefore, the choice of \( T > 0 \) depends on the distance between \( S \) and the reentrant corner. It is clear that the stress constraint may not be satisfied by any homogenized design if \( T \) is chosen too small.

The homogenized design problem is given by

\[
HP = \left\{ \inf \{ \mathcal{R}(B) \} : \begin{array}{l}
B \text{ in } D_\Theta, \\
f_i(B(x), \nabla \phi^H(x)) \leq T^2, i = 1, 2 \text{ for } x \in S
\end{array} \right\}.
\]

(4.15)

In what follows, it is supposed that at least one design \( B \) in \( D_\Theta \) satisfies (4.13) and (4.14).

**Theorem 4.1.** There is a design vector \( \hat{B} \) in \( D_\Theta \) for which the infimum of the homogenized design problem \( HP \) is attained.

This is demonstrated in section 4.4.

Next we present the class of locally layered microstructures for which a microstructure satisfying the requirements (I) and (II) can be identified using the information given by the optimal design \( \hat{B} \) of the homogenized design problem.

Consider a partition of the shaft cross section into the \( N \) subdomains \( \omega_k \), \( k = 1, \ldots, N \), such that \( \Omega = \bigcup_{k=1}^N \omega_k \). Here the maximum diameter of the subdomains in the partition is denoted by \( \tau_N \). We denote such a partition by \( \mathcal{P}_{\tau,N} \). Inside the \( k \)-th subdomain the stiff material is given by layers of thickness \( \varepsilon \theta_k^{1} \) separated by layers of compliant material of thickness \( \varepsilon \theta_k^{2} \), with \( \theta_k^{1} + \theta_k^{2} = 1 \). The layer normals inside \( \omega_k \) are specified by the angle \( \gamma_k \) and are given by \( n_k = (\cos \gamma_k, \sin \gamma_k) \). As before \( \theta_k^{1} \) and \( \gamma_k \) satisfy the box constraints

\[
0 \leq \theta_k^{\min} \leq \theta_k^{1} \leq \theta_k^{\max} < 1, \quad 0 \leq \gamma_k \leq 2\pi, \quad k = 1, \ldots, N.
\]

(4.16)

The characteristic function of the set occupied by material one for such a layered microgeometry is denoted by \( \chi_{\varepsilon,N} \), where \( \chi_{\varepsilon,N}^1 = 1 \) inside material one and zero outside and \( \chi_{\varepsilon,N}^2 = 1 - \chi_{\varepsilon,N}^1 \). The rapidly oscillating piecewise constant compliance for such a layered microgeometry is denoted by \( S_{\varepsilon,N} \) and

\[
S_{\varepsilon,N} = S_1 \chi_{\varepsilon,N}^1 + S_2 \chi_{\varepsilon,N}^2.
\]

The stress potential associated with a locally layered microgeometry is denoted by \( \phi_{\varepsilon,N} \) and vanishes on the boundary of the cross section. The stress potential satisfies the equilibrium equation

\[
-\text{div} \left( S_{\varepsilon,N} \nabla \phi_{\varepsilon,N} \right) = 1.
\]

(4.17)

The torsional rigidity of the cross section is given by

\[
\mathcal{R}_{\varepsilon,N} = 2 \int_{\Omega} \phi_{\varepsilon,N} \, dx_1 \, dx_2.
\]

(4.18)

Last we recall that the nonzero components of the in plane stress denoted by the vector \( \sigma_{\varepsilon,N} = (\sigma_{13}, \sigma_{23}) \) are related to the gradient of the stress potential according to

\[
\sigma_{\varepsilon,N} = R \nabla \phi_{\varepsilon,N},
\]

(4.19)

where \( R \) is the matrix corresponding to a counterclockwise rotation of \( \pi/2 \) and \( |\sigma_{\varepsilon,N}| = |\nabla \phi_{\varepsilon,N}| \).

For a given tolerance \( T \) the ultimate goal would be to identify a locally layered microstructure specified by \( S_{\varepsilon,N} \) with an acceptable torsional rigidity and stress potential satisfying the stress constraints in each of the materials over the prescribed set \( S \) given by

\[
\chi_{1}^{\varepsilon,N}(x) |\nabla \phi_{\varepsilon,N}(x)| \leq T \quad \text{and} \quad \chi_{2}^{\varepsilon,N}(x) |\nabla \phi_{\varepsilon,N}(x)| \leq T.
\]

(4.20)
In what follows we show that it is possible to enforce these stress constraints in a controlled asymptotic fashion and simultaneously construct a locally layered microstructure with torsional rigidity close to \( \mathcal{R}(\hat{\mathcal{B}}) \).

**Theorem 4.2.** Identification of graded microstructure.

For any given \( t > T \) and small number \( \delta > 0 \), one can construct a partition \( \mathcal{P}_{\tau N_0} \) and locally layered microstructure specified by \( S^{\varepsilon_0, N_0} \) for which the part of \( S \) over which the constraints

\[
\chi_1^{\varepsilon_0, N_0}(x)|\nabla \phi^{\varepsilon_0, N_0}(x)| \leq t \quad \text{and} \quad \chi_2^{\varepsilon_0, N_0}(x)|\nabla \phi^{\varepsilon_0, N_0}(x)| \leq t
\]

are violated has measure (area) less than \( \delta \) and

\[
|R^{\varepsilon_0, N_0} - \mathcal{R}(\hat{\mathcal{B}})| < \delta,
\]

and

\[
\int_{\Omega} (1 - \chi_1^{\varepsilon_0, N_0}) \, dx_1 \, dx_2 \leq \Theta \times (Area \, of \, \Omega) + \delta.
\]

Inside each subdomain \( \omega^k \) associated with the partition \( \mathcal{P}_{\tau N_0} \) the local layer directions and area fractions are determined from the optimal homogenized design \( \hat{\mathcal{B}} = (\hat{\theta}, \hat{\gamma}) \) through the averages given by

\[
\hat{\theta}^k = \frac{1}{Area \, of \, \omega^k} \times \int_{\omega^k} \hat{\theta}(x) \, dx_1 \, dx_2,
\]

\[
\hat{\gamma}^k = \frac{1}{Area \, of \, \omega^k} \times \int_{\omega^k} \hat{\gamma}(x) \, dx_1 \, dx_2.
\]

The systematic way in which the partition \( \mathcal{P}_{\tau N_0} \) is chosen is provided in remark 4.7 of section 4.5. Taken together theorems 4.1 and 4.2 provide an inverse homogenization method for identifying locally layered microstructures that satisfy pointwise stress constraints while delivering a torsional rigidity close to that given by the optimal design \( \hat{\mathcal{B}} \) for the homogenized design problem.

### 4.2 Computational Approach to the Homogenized Design Problem

In the computational examples we enforce the stress constraint by adding a penalty term to the torsional rigidity and minimize

\[
L = -\mathcal{R}(\mathcal{B}) + l \int_{\Omega} (f_1(\mathcal{B}(x), \nabla \phi^H))^p \, dx, \quad i = 1, 2
\]

over all design vectors \( \mathcal{B} \) in \( D_\Theta \) where \( l > 0 \) and \( \phi^H \) satisfies

\[
-div \left( S^E(\mathcal{B}) \nabla \phi^H \right) = 1
\]

and vanishes at the boundary. The computational examples provided here will be carried out for a domain with reentrant corners of interior angle \( 3\pi/2 \). In view of the strength of the associated singularity at the reentrant corners the power “\( p \)” appearing in the penalty term is chosen to be less than 3. The existence of a minimizing design \( \hat{\mathcal{B}} \) for this problem is guaranteed by the following theorem.

**Theorem 4.3.** There exists a design vector \( \hat{\mathcal{B}} \) in \( D_\Theta \) for which the infimum of (4.26) is obtained.

This theorem is established in section 4.4.

As before we use the information given in the optimal design \( \hat{\mathcal{B}} \) of (4.26) to construct a locally layered microstructure for which we have control of the pointwise stresses and for which the torsional rigidity is close to that of the optimal design for (4.26). This is formalized in the following theorem.
Theorem 4.4. Identification.
Given the optimal design $\hat{B} = (\hat{\theta}_1, \hat{\gamma})$ for (4.26) the associated stress potential is denoted by $\hat{\phi}^H$ and consider the sets

$$A_T^\delta = \{ x \in \Omega \text{ for which } f_i(\hat{B}(x), \nabla \hat{\phi}^H) \leq T^2 \}. \quad (4.28)$$

For a prescribed tolerance $\delta > 0$ and $t > T$ one can construct a partition $\mathcal{P}_{\tau N_0}$ and locally layered microstructure specified by $S^{\varepsilon_0 N_0}$ for which the part of $A_T^\delta$ over which the constraints

$$\chi_1^{\varepsilon_0 N_0}(x) |\nabla \phi^{\varepsilon_0 N_0}(x)| \leq t \quad \text{and} \quad \chi_2^{\varepsilon_0 N_0}(x) |\nabla \phi^{\varepsilon_0 N_0}(x)| \leq t \quad (4.29)$$

are violated has measure (area) less than $\delta$ and

$$|\mathcal{R}^{\varepsilon_0 N_0} - \mathcal{R}(\hat{B})| < \delta, \quad (4.30)$$

and

$$\int_{\Omega} (1 - \chi_1^{\varepsilon_0 N_0}) \, dx_1 \, dx_2 \leq \Theta \times (\text{Area of } \Omega) + \delta. \quad (4.31)$$

Inside each subdomain $\omega^k$ associated with the partition $\mathcal{P}_{\tau N_0}$ the local layer directions and area fractions are determined from the optimal homogenized design $\hat{B} = (\hat{\theta}_1, \hat{\gamma})$ through the averages given by (4.24) and (4.25).

It is noted that this theorem follows from the same arguments used to justify theorem 4.2.

The macrostress modulation functions (4.11) and (4.12) are discontinuous at $\theta_i = 0$. This is consistent with the fact that the stress amplification due to the presence of a second phase can persist even though only an infinitesimal amount of it is present. Since the objective function is differentiable on $0 < \theta_1^{\min} \leq \theta_1 \leq \theta_1^{\max} < 1$ the augmented objective function defined by (4.26) is optimized using a straightforward gradient minimization algorithm. For our computations we choose $\theta_1^{\min} = 0.01$ and $\theta_1^{\max} = 0.99$. To compute sensitivities we introduce the adjoint field $\lambda$. Here $\lambda$ is the solution of

$$-\text{div} \left( S^E(B) \nabla \lambda \right) = 1 + l \text{div} \left( 2p(Q_i(B) \nabla \phi^H \cdot \nabla \phi^H)^{p-1} Q_i(B) \nabla \phi^H \right) \quad (4.32)$$

where $1 \leq p < 3$ and $\lambda = 0$ on the boundary. For $\eta << 1$ the change in the stress potential $\phi^H$ due to small local perturbations $\eta \hat{\theta}_1, \eta \hat{\gamma}$ in the thickness and direction of the layers is written as $\hat{\phi}$ and

$$-\text{div} \left( S^E(B) \nabla \hat{\phi} \right) = \text{div} \left( (\partial_{\theta_1} S^E(B) \hat{\theta}_1 + \partial_\gamma S^E(B) \hat{\gamma}) \nabla \phi^H \right) \quad (4.33)$$

where $\hat{\phi} = 0$ on the boundary. The first variation with respect to the design variables $\theta_1$ and $\gamma$ gives to lowest order

$$\Delta L = -\int_{\Omega} \hat{\phi} \, dx + \int_{\Omega} p(Q_i(B) \nabla \phi^H \cdot \nabla \phi^H)^{p-1}(\partial_{\theta_1} Q_i(B) \hat{\theta} + \partial_\gamma Q_i(B) \hat{\gamma}) \nabla \phi^H \cdot \nabla \phi^H \, dx + \int_{\Omega} 2p(Q_i(B) \nabla \phi^H \cdot \nabla \phi^H)^{p-1} Q_i(B) \nabla \phi^H \cdot \nabla \phi \, dx. \quad (4.34)$$

The choice of $\hat{\theta}_1$ and $\hat{\gamma}$ that renders $\Delta L$ the most negative is given by

$$\hat{\theta}_1 = -\partial_{\theta_1} S^E(B) \nabla \lambda \nabla \phi^H - 2l p(Q_i(B) \nabla \phi^H \cdot \nabla \phi^H)^{p-1} \partial_{\theta_1} Q_i(B) \nabla \phi^H \cdot \nabla \phi^H \quad (4.35)$$

The continuity constraints on $\theta_1(x), \gamma(x)$ expressed by (4.3) are enforced by the way in which the design variables are initialized and updated. The local average of a scalar function $f$ over the disk of
radius $R$ centered at $p$ is denoted by $<f>_R(p)$. For given fields $\theta_1, \gamma$ satisfying the resource and box constraints (4.1) and (4.2) the initial choice of design variables $\theta_1^0, \gamma^0$ are given by

$$\theta_1^0 = \langle \theta_1 \rangle_R(x) \quad \text{and} \quad \gamma^0 = \langle \gamma \rangle_R(x).$$

At the $n$th step we suppose that $\theta_1$ and $\gamma$ are given and we solve for $\phi$ and $\lambda$ using the system of equations (4.27) and (4.32). The design variables $\theta_1$ and $\gamma$ are updated according to

$$\theta_{1,new} = \langle \theta_1 + \eta \tilde{\theta}_1 \rangle_R(x) \quad \text{and} \quad \gamma_{new} = \langle \gamma + \eta \tilde{\gamma} \rangle_R(x)$$

were $\tilde{\theta}_1$ and $\tilde{\gamma}$ are given by (4.35). Because the updated functions are given by averages of bounded functions it is easily seen that they satisfy (4.3) for $\alpha = 1$ and for some non-negative constant $K$ independent of $x$.

The algorithm is guaranteed to converge due to the monotonic change of the objective under our choice of perturbation. The use of local averaging in the update scheme is similar to the use of filters in topology optimization, see [5] and [4].

For points near the boundary a difficulty arises when defining the averages. This is dealt with by extending $\theta_1$ and $\gamma$ to the slightly larger domain $\Omega_R = \{x \in \mathbb{R}^2; \text{dist}(x, \Omega) \leq R\}$. The particular form of extension is up to the designer. Possibilities include setting $\theta_1 = 1$ and $\gamma = 0$ in $\Omega_R \setminus \Omega$ or reflection of $\theta_1, \gamma$ across the boundary of $\Omega$ into $\Omega_R$. In the discretized problem used for the simulations we allow $\theta_1$ and $\gamma$ to take constant values inside each element and define $\langle \theta_1 \rangle_R$ and $\langle \gamma \rangle_R$ to be the averages of $\theta_1$ and $\gamma$ over neighboring elements.

### 4.3 Numerical Implementation for the X-shaped and L-shaped Cross Sections

The first set of computational examples are carried out for an “X” shaped domain. All interior angles for the reentrant corners are fixed at $3\pi/2$ radians. The shear stiffness of material one is assigned the value $G_1 = 1 \text{ GPa}$ and the shear stiffness of material two is assigned the value $G_2 = 2 \text{ GPa}$. For these choices $S_1 = 1/(2G_1) = 0.5$ and $S_2 = 1/(2G_2) = 0.25$. All of the design optimizations presented here are carried out with the area fraction of the compliant material held near 30% of the total area of the shaft cross section.

In figure 4.2 a plot of the local density $\hat{\theta}_1(x)$ of material one is given for an optimal design minimizing (4.26) subject to the penalization on $\int (f_i)$, i.e., $i = 1$ and $p = 1$ in (4.26). The darkest regions correspond to zones of composite containing the highest density of the compliant material, i.e., $\hat{\theta}_1 = 0.99$. The lightest zones correspond to regions where $\hat{\theta}_1 = 0.01$. In this design the most compliant material is placed next to the reentrant corners. In figure 4.3 the arrows representing the local layer normals $(\cos \hat{\gamma}(x), \sin \hat{\gamma}(x))$ are plotted for the optimal homogenized design.

In the next example we optimize for torsional rigidity only. The resulting design is referred to as design 1. The plot of $\hat{\theta}_1$ for this design is given in figure 4.4. Here the lightest region corresponds to the stiffest possible effective material with density $\hat{\theta}_1 = 0.01$. The darkest corresponds to the most compliant material with $\hat{\theta}_1 = 0.99$. As expected this design ignores the stress concentration at the reentrant corners and the stiffest material surrounds the compliant material in order to impart the greatest torsional rigidity to the structure. In the next example the torsional rigidity is optimized in the presence of an integral penalization $\int (f_j)^2$, i.e., $i = 1$ and $p = 2$ for the Lagrangian in (4.26). The resulting design is referred to as design 2. The plot of $\hat{\theta}_1$ for this design is given in figure 4.5. For this case the more compliant material surrounds the stress concentration at the reentrant corners. In the
final example the torsional rigidity is optimized in the presence of an integral penalization \( \int (f_2)^2 \), i.e., \( i = 2 \) and \( p = 2 \) for the Lagrangian in (4.26). The resulting design is referred to as design 3. The plot of \( \hat{\theta}_1 \) for this design is given in figure 4.6. It is seen that the more compliant material surrounds the stress concentration at the reentrant corners. The associated torsional rigidities for each of these cases are listed in table 4.1. It is seen from the table that the torsional rigidity drops for the penalized designs.

The contour plot of the macrostress modulation function \( f_1 \) for design 1 is given in figure 4.7. Figure 4.8 gives the contour plot for \( f_1 \) in design 2. When comparing designs 1 and 2 it is clear from figures 4.7 and 4.8 that design 2 provides a significant reduction in the size of the over stressed zone \( f_1 \geq 0.3 \).

It is pointed out that theorem 4.2 provides the method for constructing a locally layered material from the data given in design 2. The choice of partition \( P_{\varepsilon,N} \) used in the construction can be obtained from any initially chosen partition after sufficient refinement of the initial partition; this is discussed in Section 6. To fix ideas we choose a tolerance \( \delta = 1/1000 \) and \( t = 0.301 \). Then theorem 4.2 together with remark 4.7 in section 4.5 shows how to construct a locally layered composite with layer thicknesses on a length scale \( \varepsilon_0 > 0 \) and torsional rigidity \( \mathcal{R}^{\varepsilon_0,N_0} \) for which

\[
|\mathcal{R}^{\varepsilon_0,N_0} - 0.61| < 1/1000
\]  

and for which the magnitude of the in plane stress in material one lies below 0.301 for all points in the region \( f_1 < 0.3 \) of figure 4.8, with the possible exception of a subset of points of area less than 1/1000.

The contour plot of the macrostress modulation function \( f_2 \) is presented in figure 4.9 for design 1. Figure 4.10 gives the contour plot of \( f_2 \) for design 3. An inspection of figures 4.9 and 4.10 shows that design 3 provides a significant reduction in the size of the over stressed zone \( f_2 \geq 0.1 \) when compared to design 1.

Last we consider the “L” shaped domain. In the first example for the “L” shaped domain we optimize for torsional rigidity only. The resulting design is referred to as design 4. The plot of \( \hat{\theta}_1 \) for this design is given in figure 4.11. Here the lightest region corresponds to the stiffest possible effective material with density \( \hat{\theta}_1 = 0.01 \). The darkest corresponds to the most compliant material with \( \hat{\theta}_1 = 0.99 \). As before this design ignores the stress concentration at the reentrant corners and the stiffest material surrounds the compliant material in order to impart the greatest torsional rigidity to the structure. In the next example the torsional rigidity is optimized in the presence of the integral penalization \( \int (f_2)^2 \), i.e., for the Lagrangian in (4.26). The resulting design is referred to as design 5. The plot of \( \hat{\theta}_1 \) for this design is given in figure 4.12. It is seen that the more compliant material surrounds the stress concentration at the reentrant corners. The contour plot of the macrostress modulation function \( f_2 \) is plotted in figure 4.13 for design 4. Figure 4.14 gives the contour plot of \( f_2 \) for design 5. Inspection of figures 4.13 and 4.14 shows that design 5 provides a significant reduction in the size of the over stressed zone \( f_2 \geq 0.1 \) when compared to design 4. We point out that the torsional rigidity for design 4 is 3.9 while for design 5 it drops by almost half to 2.0. The examples show that the optimized designs for the “L” shaped domain exhibit the same trends as those for the “X” shaped domain.

### 4.4 The Optimal Design for the Homogenized Design Problem

In this section we proceed using the direct method of the calculus of variations to show that there is an optimal design for the homogenized design problem presented in section 4.1. One starts by considering a minimizing sequence \( \{B_n\}_{n=1}^{\infty} \) for the homogenized design problem. The associated sequence of compliance tensors is denoted by \( \{S^E(B_n(x))\}_{n=1}^{\infty} \) and the stress potentials \( \{\phi_n^H\}_{n=1}^{\infty} \) vanish on the boundary of the cross section and are solutions of

\[
-\text{div} \left(S^E(B_n)\nabla \phi_n^H\right) = 1
\]  

(4.39)
satisfying the stress constraints
\[ f_i(B_n, \nabla \phi_n^H) \leq T^2, \text{ for } i = 1, 2 \] (4.40)
over the set \( S \) and
\[ HP = \lim_{n \to \infty} 2 \int_\Omega \phi_n^H \, dx_1 \, dx_2. \] (4.41)

Since \( \{B_n(x)\}_{n=1}^\infty \) is an equicontinuous family of functions over the closure of \( \Omega \) one readily deduces that there is a subsequence, also denoted by \( \{B_n(x)\}_{n=1}^\infty \), converging uniformly in \( \Omega \) to a design \( \hat{B} \) in \( D_\Theta \). This delivers the convergence
\[ \lim_{n \to \infty} S^E(B_n(x)) = S^E(\hat{B}(x)) \quad \text{and} \]
\[ \lim_{n \to \infty} f_i(B_n(x), \nu) \geq f_i(\hat{B}(x), \nu) \quad i = 1, 2 \] (4.42)
for every point \( x \) in the domain. From the theory of G-convergence [31] and H-convergence [27] one has that the sequence \( \{\phi_n^H\}_{n=1}^\infty \) converges weakly in the Sobolev space \( W^{1,2}_0(\Omega) \) to the stress potential \( \hat{\phi}^H \) associated with \( S^E(\hat{B}) \) where
\[ -\text{div} \left( S^E(\hat{B}) \nabla \hat{\phi}^H \right) = 1 \] (4.43)
and
\[ \lim_{n \to \infty} 2 \int_\Omega \phi_n^H \, dx_1 \, dx_2 = 2 \int_\Omega \hat{\phi}^H \, dx_1 \, dx_2. \] (4.44)

To conclude the proof one checks to see if the homogenized stress constraints given by (4.13) and (4.14) are satisfied by the stress associated with the design \( \hat{B} \). Since the sequence \( \{S^E(B_n(x))\}_{n=1}^\infty \) converges pointwise to \( S^E(\hat{B}(x)) \) (see [31]) the sequence of gradients \( \{\nabla \phi_n^H\}_{n=1}^\infty \) converge strongly in \( L^2(\Omega)^2 \) to \( \nabla \hat{\phi}^H \), see [31]. Passing to a subsequence if necessary, also denoted by \( \{\nabla \phi_n^H\}_{n=1}^\infty \), it follows that this subsequence converges pointwise to \( \nabla \hat{\phi}^H \). From this one deduces that
\[ T^2 \geq \lim_{n \to \infty} f_i(B_n, \nabla \phi_n^H) \geq f_i(\hat{B}, \nabla \hat{\phi}^H), \text{ for } i = 1, 2 \] (4.45)
for almost every point and theorem 4.1 is established.

The proof of theorem 4.3 follows the same steps given in the proof of theorem 4.1. As before one concludes that the minimizing sequence \( \{B_n(x)\}_{n=1}^\infty \) of designs for (4.26) converge uniformly to the limit \( \hat{B} \) where \( \hat{B} \) is in \( D_\Theta \). Here the associated stress potentials \( \{\phi_n^H\}_{n=1}^\infty \) satisfy
\[ \lim_{n \to \infty} 2 \int_\Omega \phi_n^H \, dx_1 \, dx_2 = 2 \int_\Omega \hat{\phi}^H \, dx_1 \, dx_2 = R(\hat{B}) \] (4.46)
and the pointwise convergence
\[ \lim_{n \to \infty} \nabla \phi_n^H(x) = \nabla \hat{\phi}^H(x), \text{ a.e.} \] (4.47)
where
\[ -\text{div} \left( S^E(\hat{B}) \nabla \hat{\phi}^H \right) = 1. \] (4.48)
Last, Fatou’s lemma gives
\[ \int_\Omega f_i(\hat{B}(x), \nabla \hat{\phi}^H)^p \, dx \leq \lim_{n \to \infty} \inf \int_\Omega (f_i(B_n(x), \nabla \phi_n^H))^p \, dx, \quad i = 1, 2 \] (4.49)
and theorem 4.3 follows.
4.5 Identifying Locally Layered Microgeometry with Desirable Strength and Stiffness Properties

In this section theorem 4.2 is established. The proof is based on two steps. In the first step a version of the identification theorem is established (theorem 4.6) for the case when the design vector $B(x)$ takes piecewise constant values. In the next step theorem 4.2 is established by making use of a sequence of piecewise constant approximations to the optimal design vector $\hat{B}$.

Consider a partition of the shaft cross section $\mathcal{P}_{N}$ with the subsets in the partition denoted by $\omega_{N}^{k}$, $k = 1, \ldots, N$. We follow the standard convention in the theory of finite elements and take the subsets in the partition to be open such that the union of their closures is equal to the closure of the set $\Omega$ describing the cross section. Denoting the piecewise constant design vector by $B_{N}(x)$ we suppose that it takes the constant values $(\theta_{1N}^{k}, \gamma_{1N}^{k})$ for $x$ inside each subdomain $\omega_{N}^{k}$. Here $\theta_{1N}^{k}$ and $\gamma_{1N}^{k}$ satisfy the box constraints given by (4.16). The associated compliance tensor $S^{E}(B_{N})$ is piecewise constant and the stress potential $\phi_{N}$ vanishes on the boundary and is the solution of

$$-\text{div} \left( S^{E}(B_{N}) \nabla \phi_{N} \right) = 1.$$

(4.50)

Suppose we are given that $\nabla \phi_{N}$ satisfies the stress constraints given by

$$f_{i}(B_{N}, \nabla \phi_{N}) \leq \tau^{2} \quad \text{for} \quad i = 1, 2 \quad \text{and} \quad x \quad \text{in} \quad \omega,$$

(4.51)

where $\omega$ is a subset of the cross section. Here the distance between any point inside $\omega$ and the boundary of the cross section is greater than some fixed positive number. Next consider the locally layered microstructure with the thickness of the stiff layers and compliant layers given by $\varepsilon \theta_{1N}^{k}$ and $\varepsilon \theta_{2N}^{k}$ respectively in $\omega_{N}^{k}$. The layer normals are specified by $\gamma_{1N}^{k}$ in $\omega_{N}^{k}$. The associated piecewise constant compliance is given by $S^{\varepsilon, N} = S_{1}\chi_{1}^{\varepsilon, N} + S_{2}\chi_{2}^{\varepsilon, N}$. The stress potential in the shaft cross section filled with locally layered material is denoted by $\phi^{\varepsilon, N}$. The stress potential vanishes on the boundary and is a solution of

$$-\text{div} \left( S^{\varepsilon, N} \nabla \phi^{\varepsilon, N} \right) = 1.$$

(4.52)

**Definition 4.5.** For $t \geq 0$ we introduce the distribution function $\lambda_{i}^{\varepsilon, N}(t, \omega)$ which gives the Lebesgue measure (area) of the set of points in $\omega$ where $\chi_{i}^{\varepsilon, N}|\nabla \phi^{\varepsilon, N}| > t$, $i = 1, 2$.

We now establish the following theorem.

**Theorem 4.6.** Suppose that the homogenized stress constraint (4.51) holds, then on passage to a subsequence if necessary, the sequence of stress potentials $\{\phi^{\varepsilon, N}\}_{\varepsilon > 0}$ has the following two properties given by

$$\lim_{\varepsilon \to 0} \int_{\Omega} \phi^{\varepsilon, N} d\Omega = 2 \int_{\Omega} \phi_{N} d\Omega$$

(4.53)

and

$$\lim_{\varepsilon \to 0} \lambda_{i}^{\varepsilon, N}(t, \omega) = 0 \quad \text{for} \quad t > \tau.$$

(4.54)

Note here that (4.54) states that for any $t > \tau > 0$ that the area of the part of $\omega$ over which

$$\chi_{1}^{\varepsilon, N}|\nabla \phi^{\varepsilon, N}| > t \quad \text{and} \quad \chi_{2}^{\varepsilon, N}|\nabla \phi^{\varepsilon, N}| > t$$

(4.55)

vanishes as $\varepsilon \to 0$.

**Proof of theorem 4.6.**

The sequence $\{S^{\varepsilon, N}\}_{\varepsilon > 0}$ associated with locally layered geometries converge in homogenization to $S^{E}(B_{N})$ see [26]. Consequently the sequence of potentials $\{\phi^{\varepsilon, N}\}_{\varepsilon > 0}$ converge weakly in the Sobolev
space $W^{1,2}_0(\Omega)$ to $\phi^N$ and (4.53) follows. To establish (4.54) of theorem 4.6 we introduce the characteristic function $\chi_{i,t}^{\varepsilon,N}$ of the set of points in $\Omega$ where $\chi_{i,t}^{\varepsilon,N}|\nabla \phi_{t}^{\varepsilon,N}| > t$, $i = 1, 2$. Here

$$\chi_{i,t}^{\varepsilon,N}(t, \omega) = \int \chi_{i,t}^{\varepsilon,N} dx_1 dx_2.$$  \hfill (4.56)

From the theory of weak convergence [10] one passes to a subsequence if necessary to assert the existence of a density $\theta_{i,t}^{N}$ for which,

$$\lim_{\varepsilon \to 0} \chi_{i,t}^{\varepsilon,N}(t, \omega) = \int \theta_{i,t}^{N} dx_1 dx_2.$$  \hfill (4.57)

Here, $0 \leq \theta_{i,t}^{N} \leq 1$. In physical terms $\theta_{i,t}^{N}$ can be thought of as giving the distribution of states for the stress in the homogenized composite. The derivative of $\theta_{i,t}^{N}$ with respect to $t$ gives the density of states. For any point $x$ inside the cross section we introduce the sequence of squares centered at $x$ with side length $\ell_j = 1/j$, $j = 1, 2, \ldots$ denoted by $Q(x, j)$. For $j$ large enough the squares are contained inside $\omega$. We test the microstructure inside the squares by imposing two linearly independent unit loads given by $e^1 = (1, 0)$ and $e^2 = (0, 1)$ and track the stress fluctuations inside the square as $\varepsilon$ tends to zero. Mathematically this is done by keeping track of the $Q(x, j)$ periodic stress potentials $w_{m}^{\varepsilon,j,N}$ that solve

$$\text{div} \left( S^{\varepsilon,N} (\nabla w_{m}^{\varepsilon,j,N} + e^m) \right) = 0, \text{ for } m = 1, 2.$$  \hfill (4.58)

For $y$ in $Q(x, j)$ we introduce the fluctuation matrix $Q_{mn}^{i,j,N}(y)$ defined by

$$Q_{mn}^{i,j,N}(y) = \chi_{i}^{\varepsilon,N}(y)(\nabla w_{m}^{\varepsilon,j,N}(y) + e^m) \cdot (\nabla w_{n}^{\varepsilon,j,N}(y) + e^n).$$  \hfill (4.59)

From Lemma 3.7 of [15] one has

$$t^2 \theta_{i,t}^{N}(x) \leq M_{i}^{*,N}(x) \nabla \phi^N(x) \cdot \nabla \phi^N(x), \text{ a.e.},$$  \hfill (4.60)

where the tensor $M_{i}^{*,N}(x)$ is defined by

$$M_{i}^{*,N}(x) = \lim_{j \to \infty} \lim_{\varepsilon \to 0} \frac{1}{|Q(x, j)|} \int Q(x, j) \chi_{i,t}^{\varepsilon,N}(y) Q_{mn}^{i,j,N}(y) dy_1 dy_2.$$  \hfill (4.61)

We now develop an upper bound on $M_{i}^{*,N}(x)$ that is given in terms of $\theta_{i,t}^{N}(x)$ and $f_i(\mathcal{B}_N, \nabla \phi^N(x))$. It is supposed that $x$ lies in one of the subsets of the partition. This is true for almost every point in the cross section. Without loss of generality suppose this subset is $\omega^k_N$. For $\ell_j$ sufficiently small $Q(x, j)$ is compactly contained inside $\omega^k_N$ and we apply the corrector theory given in [27] to easily deduce that

$$\nabla w_{m}^{\varepsilon,j,N}(y) + e^m = P^{\varepsilon,k,N} (y) e^m + r^{\varepsilon,k,N},$$  \hfill (4.62)

where

$$r^{\varepsilon,k,N} \to 0$$  \hfill (4.63)

in mean square over $Q(x, j)$. For $y$ in $Q(x, j)$, the corrector matrix is given by

$$P^{\varepsilon,k,N}(y) = \chi_{1}^{\varepsilon,N}(y) R(\gamma^k_{N}) \Lambda^1(\theta_{1}^{k,N}) R^T(\gamma^k_{N}) + \chi_{2}^{\varepsilon,N}(y) R(\gamma^k_{N}) \Lambda^2(\theta_{1}^{k,N}) R^T(\gamma^k_{N}).$$  \hfill (4.64)

From (4.61)–(4.64) one sees that

$$M_{i}^{*,N}(x) = \lim_{j \to \infty} \lim_{\varepsilon \to 0} \frac{1}{|Q(x, j)|} \int Q(x, j) \chi_{i,t}^{\varepsilon,N}(y) Q_{i}(\mathcal{B}_N) dy_1 dy_2 i = 1, 2,$$  \hfill (4.65)
where \( Q_i(B_i), \ i = 1, 2 \) are given by (4.8) and (4.9).

In order to facilitate the exposition we provide an explicit formula for the characteristic functions \( \chi_{\epsilon,N}^{i} \) in terms of the local layer normal and volume fraction. Let \( a \) be a number in \([0,1]\) and define periodic functions on \([0,1]\) denoted by \( \chi_1(a,s) \) and \( \chi_2(a,s) \) such that \( \chi_1(a,s) = 1 \) for \( 0 \leq s < a \), \( \chi_1(a,s) = 0 \) for \( a \leq s \leq 1 \) and \( \chi_2(a,s) = 1 - \chi_1(a,s) \). Then for \( x \in \omega_k \), one writes \( \chi_{\epsilon,N}^{i} = \chi_i(n^k \cdot x/\epsilon) \). We apply Holder’s inequality to deduce that

\[
M^{i,N}(x) \nabla \phi^{N}(x) \cdot \nabla \phi^{N}(x) \\
\leq \lim_{j \to \infty} \lim_{\epsilon \to 0} \frac{1}{|Q(x,j)|} \int_{Q(x,j)} \chi_{\epsilon,N}^{i}(y) dy_1 dy_2 \\
\times \sup_{0 \leq s \leq 1} \left\{ \chi_i(\theta_{1}^{N}, s) Q_i(B_N) \nabla \phi^{N}(x) \cdot \nabla \phi^{N}(x) \right\} \\
= \theta_{i,t}^{N}(x) f_i(B_N, \nabla \phi^{N}(x)),
\]

(4.66)

where

\[
\theta_{i,t}^{N}(x) = \lim_{j \to \infty} \lim_{\epsilon \to 0} \frac{1}{|Q(x,j)|} \int_{Q(x,j)} \chi_{\epsilon,N}^{i}(y) dy_1 dy_2
\]

(4.67)

holds for almost every point in \( \omega \) and \( f_i(B_N,v) \) are the macrostress modulations defined by (4.11) and (4.12).

The inequality (4.60) together with (4.66) delivers the homogenization constraint

\[
\theta_{i,t}^{N}(x) \left( f_i(B_N, \nabla \phi^{N}) - t^2 \right) \geq 0, \quad i = 1, 2,
\]

(4.68)

for \( t > 0 \) and almost every \( x \) in \( \omega \).

In what follows we will denote the measure (area) of a set \( G \) by \(|G|\). The set of points in \( \omega \) for which \( \theta_{i,t}^{N}(x) > 0 \) is denoted by \( \{ \theta_{i,t}^{N} > 0 \} \) and the set of points in \( \omega \) for which \( f_i(B_N, \nabla \phi^{N}) \geq t^2 \) is denoted by \( \{ f_i \geq t^2 \} \). From (4.68) it is evident that almost every point in \( \{ \theta_{i,t}^{N} > 0 \} \) is also belongs to \( \{ f_i \geq t^2 \} \) so

\[
|\{ \theta_{i,t}^{N} > 0 \}| \leq |\{ f_i \geq t^2 \}|.
\]

(4.69)

It follows that

\[
\lim_{\epsilon \to 0} \lambda_{i}^{\epsilon,N}(t,\omega) = \int_{\omega} \theta_{i,t}^{N} dx_1 dx_2 \leq |\{ \theta_{i,t}^{N} > 0 \}|
\]

(4.70)

and from (4.69) we deduce that

\[
\lim_{\epsilon \to 0} \lambda_{i}^{\epsilon,N}(t,\omega) \leq |\{ f_i \geq t^2 \}|
\]

(4.71)

and it is clear that

\[
\lim_{\epsilon \to 0} \lambda_{i}^{\epsilon,N}(t,\omega) = 0
\]

(4.72)

if

\[
f_i(B_N, \nabla \phi^{N}) < t^2 \quad \text{for all points } x \in \omega
\]

(4.73)

and theorem 4.6 is proved.

In order to expedite the presentation we call any partition \( \mathcal{P}_{\tau,M} \) of the shaft into \( M \) subdomains with \( M > N \) a refinement of \( \mathcal{P}_{\tau,N} \) if \( \tau_N \geq \tau_M \), and if every set in the partition \( \mathcal{P}_{\tau,M} \) is a subset of a set belonging to \( \mathcal{P}_{\tau,N} \). Now for a given partition \( \mathcal{P}_{\tau,N} \) consider a sequence of refinements \( \{ \mathcal{P}_{\tau_{N_j}} \}_{j=1}^{\infty} \) such that \( \mathcal{P}_{\tau_{N_j+1}} \) is a refinement of \( \mathcal{P}_{\tau_{N_j}} \) with \( \mathcal{P}_{\tau_{N_1}} = \mathcal{P}_{\tau_N} \). Here \( \tau_{N_j} \) tends to zero as \( j \) tends to infinity. The sets belonging to \( \mathcal{P}_{\tau_{N_j}} \) are denoted by \( \omega_{k}^{N_j}, \ k = 1, \ldots, N_j \).
Recall the optimal design $\hat{\mathcal{B}}$ and let $\mathcal{B}_{N_j}$ denote the piecewise constant design vector taking values $(\theta_{N_j}^k, \gamma_{N_j}^k)$ determined by the averages
\begin{align}
\hat{\theta}_{1N_j}^k &= \frac{1}{\text{Area of } \omega_{N_j}^k} \times \int_{\omega_{N_j}^k} \hat{\theta}_1(x) dx_1 dx_2, \\
\hat{\gamma}_{N_j}^k &= \frac{1}{\text{Area of } \omega_{N_j}^k} \times \int_{\omega_{N_j}^k} \hat{\gamma}(x) dx_1 dx_2.
\end{align}
(4.74)

Associated with $\mathcal{B}_{N_j}$ is the piecewise constant compliance tensor $S^E(\mathcal{B}_{N_j})$ and stress potential $\phi_{N_j}$ that vanishes on the boundary of the cross section and satisfies
\begin{equation}
- \text{div} \left( S^E(\mathcal{B}_{N_j}) \nabla \phi_{N_j} \right) = 1.
\end{equation}
(4.76)

We consider the intersection of the set of Lebesgue points for each of the functions $\hat{\theta}_1$ and $\hat{\gamma}$. On this set $\mathcal{B}_{N_j} \to \hat{\mathcal{B}}$ as $j \to \infty$. This delivers the convergence
\begin{equation}
\lim_{j \to \infty} S^E(\mathcal{B}_{N_j}) = S^E(\hat{\mathcal{B}})
\end{equation}
(4.77)
for almost every $x$ in $\Omega$. Define $\hat{\theta}_2 = 1 - \hat{\theta}_1$ and for almost every point for which $\hat{\theta}_i(x) > 0$ one has that
\begin{equation}
\lim_{j \to \infty} f_i(\mathcal{B}_{N_j}(x), \nabla \phi_{N_j}(x)) = f_i(\hat{\mathcal{B}}(x), \nabla \phi_{H}(x)),
\end{equation}
(4.78)
otherwise over almost every point for which $\hat{\theta}_i(x) = 0$ one has
\begin{equation}
\lim_{j \to \infty} f_i(\mathcal{B}_{N_j}(x), \nabla \phi_{N_j}(x)) \geq f_i(\hat{\mathcal{B}}(x), \nabla \phi_{H}(x)) = 0.
\end{equation}
(4.79)

It follows immediately from the theory of homogenization [31, 27] that $\{\phi_{N_j}\}_{j=1}^\infty$ converges weakly in the Sobolev space $W^{1,2}_0$ to $\hat{\phi}^H$ and
\begin{equation}
\lim_{j \to \infty} \int_{\Omega} \phi_{N_j} dx_1 dx_2 = \int_{\Omega} \hat{\phi}^H dx_1 dx_2.
\end{equation}
(4.80)

Moreover since the sequence of tensors $\{S^E(\mathcal{B}_{N_j})\}_{j=1}^\infty$ converge pointwise to $S^E(\hat{\mathcal{B}})$, standard arguments show that the sequence $\{\nabla \phi_{N_j}\}_{j=1}^\infty$ converges in mean square to $\nabla \hat{\phi}^H$. On passing to a subsequence if necessary one may assume that the sequence $\{\nabla \phi_{N_j}\}_{j=1}^\infty$ converges almost everywhere to $\nabla \hat{\phi}^H$.

We partition the set $\mathcal{S}$ into two subsets $\mathcal{S}_0^0$ and $\mathcal{S}_i^+$ where $\hat{\theta}_i = 0$ on $\mathcal{S}_0^0$ and $\hat{\theta}_i > 0$ on $\mathcal{S}_i^+$. Collecting observations one readily sees that
\begin{equation}
\lim_{j \to \infty} f_i(\mathcal{B}_{N_j}(x), \nabla \phi_{N_j}(x)) = f_i(\hat{\mathcal{B}}(x), \nabla \hat{\phi}^H(x))
\end{equation}
(4.81)
for almost every $x$ in $\mathcal{S}_i^+$ and
\begin{equation}
\lim_{j \to \infty} f_i(\mathcal{B}_{N_j}(x), \nabla \phi_{N_j}(x)) \geq f_i(\hat{\mathcal{B}}(x), \nabla \hat{\phi}^H(x)) = 0
\end{equation}
(4.82)
for almost every $x$ in $\mathcal{S}_0^0$.  

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Next consider the sequence of piecewise locally layered microstructures associated with $\mathcal{S}^E(\mathcal{B}_{N_j})$ constructed according to the hypotheses of theorem 4.6. The sequence of stress potentials for these microstructures are denoted by $\{\phi^{\varepsilon,N_j}\}_{j=1}^{\infty}$. From theorem 4.6 and (4.80) it follows immediately that

$$\lim_{j \to \infty} \int_{\Omega} \phi^{\varepsilon,N_j} \, dx \, dx_2 = \int_{\Omega} \phi^{H} \, dx \, dx_2 = \mathcal{R}(\hat{B}).$$

(4.83)

And standard arguments show that for any subset $C$ of $\Omega$

$$\lim_{j \to \infty} \int_{C} \chi^\varepsilon_{N_j} \, dx \, dx_2 = \lim_{j \to \infty} \int_{C} \theta_j \, dx \, dx_2 = \int_{C} \hat{\theta}_j \, dx \, dx_2.$$

(4.84)

In order to finish the proof of theorem 4.2 it remains to show that for $t > T$ that the associated sequence of distribution functions $\lambda^\varepsilon_{N_j}(t,\mathcal{S})$ satisfy

$$\lim_{j \to \infty} \lambda^\varepsilon_{N_j}(t,\mathcal{S}) = 0, \quad i = 1, 2. \quad (4.85)$$

We write $\mathcal{S} = \mathcal{S}_i \cup \mathcal{S}_i^+$ and note that

$$\lim_{j \to \infty} \lambda^\varepsilon_{N_j}(t,\mathcal{S}) = \lim_{j \to \infty} \lambda^\varepsilon_{N_j}(t,\mathcal{S}_i^0) + \lim_{j \to \infty} \lambda^\varepsilon_{N_j}(t,\mathcal{S}_i^+), \quad i = 1, 2. \quad (4.86)$$

We then observe that the inequality $\chi^\varepsilon_{N_j} \leq \chi^\varepsilon_{N_j}$ together with (4.84) gives

$$\lim_{j \to \infty} \lambda^\varepsilon_{N_j}(t,\mathcal{S}_i^0) = 0. \quad (4.87)$$

We choose $\tau$ so that $T < \tau < t$. Setting

$$A^7_{N_j} = \{x \in \mathcal{S}_i^+; f_i(\mathcal{B}_{N_j}(x),\nabla \phi^{N_j}(x)) > \tau^2\}$$

(4.88)

it is evident from (4.81) and

$$f_i(\hat{\mathcal{B}}(x),\nabla \phi^{H}(x)) \leq T^2, \quad i = 1, 2 \quad (4.89)$$

that $\lim_{j \to \infty} |A^7_{N_j}| = 0$ for $\tau > T$. The points in $\mathcal{S}_i^+$ not in $A^7_{N_j}$ are denoted by $\mathcal{S}_i^+ \setminus A^7_{N_j}$. On this set $f_i(\mathcal{B}_{N_j}(x),\nabla \phi^{N_j}(x))) \leq \tau^2$ and from theorem 4.6 we deduce that

$$\lim_{j \to \infty} \lambda^\varepsilon_{N_j}(t,\mathcal{S}_i^+ \setminus A^7_{N_j}) = 0. \quad (4.90)$$

Last it is evident that $\lambda^\varepsilon_{N_j}(t,A^7_{N_j}) \leq |A^7_{N_j}|$ and (4.85) follows after taking limits, since

$$\lambda^\varepsilon_{N_j}(t,\mathcal{S}_i^+) = \lambda^\varepsilon_{N_j}(t,A^7_{N_j}) + \lambda^\varepsilon_{N_j}(t,\mathcal{S}_i^+ \setminus A^7_{N_j})$$

(4.91)

and theorem 4.2 is established.

**Remark 4.7.** The proof of theorem 4.2 contains the algorithm for selecting the partition used in the construction of a locally layered microstructure that satisfies the design requirements given by (4.21), (4.22) and (4.23). Indeed one can choose any initial partition denoted by $\mathcal{P}_{\tau,N}$ and consider the sequence of refinements $\{\mathcal{P}_{\tau,N_j}\}_{j=1}^{\infty}$ where $\mathcal{P}_{\tau,N_1} = \mathcal{P}_{\tau,N}$ and

$$\lim_{j \to \infty} \tau^N = 0. \quad (4.92)$$

For given tolerances $t > T$ and $\delta > 0$ it follows from (4.83), (4.84) and (4.85) that there exist a sufficiently refined partition $\mathcal{P}_{\tau,j}$, for which one can choose a locally layered microstructure on a sufficiently fine length scale $\varepsilon_0$ that satisfies the design requirements (4.21), (4.22) and (4.23).
4.6 Extension to Two and Three Dimensional Elastic Problems

The numerical method presented here can be applied to the design of locally layered microstructures for fully three dimensional linear elastic problems. This can be justified following the methods developed in this chapter. The only technical modification necessary to justify the method for the three dimensional case is to replace the convergence result described by (4.62) and (4.63) with the analogous one suitable for the system of linearly elasticity. Such a convergence result follows directly from the work of [6].

<table>
<thead>
<tr>
<th>Design #</th>
<th>Stress Constraint</th>
<th>$S_1$-Volume Fraction</th>
<th>Torsional Rigidity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>None</td>
<td>30.8%</td>
<td>0.82</td>
</tr>
<tr>
<td>2</td>
<td>$\mathcal{J}(f_1)^2$</td>
<td>32.1%</td>
<td>0.61</td>
</tr>
<tr>
<td>3</td>
<td>$\mathcal{J}(f_2)^2$</td>
<td>30.1%</td>
<td>0.62</td>
</tr>
</tbody>
</table>

FIGURE 4.2. Density distribution of compliant material in X-shaped cross section optimized for torsional rigidity with a $p = 1$ integral penalization on $f_1$. The darkest regions correspond to the most compliant material the lightest region corresponds to the location of the stiffest material.
FIGURE 4.3. Local layer directions and level lines of stress potential inside the X-shaped cross section optimized for torsional rigidity with a $p = 1$ integral penalization on $f_1$.

FIGURE 4.4. Design 1. Plot of the density distribution of compliant material in X-shaped shaft cross section optimized for torsional rigidity only.
FIGURE 4.5. Design 2. Density distribution of compliant material in X-shaped cross section optimized for torsional rigidity with $p = 2$ integral penalty on $f_1$.

FIGURE 4.6. Design 3. Density distribution of compliant material in X-shaped cross section optimized for torsional rigidity with $p = 2$ integral penalty on $f_2$. 
FIGURE 4.7. Contour plot of $f_1$ for design 1.

FIGURE 4.8. Contour plot of $f_1$ for design 2.

FIGURE 4.9. Contour plot of $f_2$ for design 1.
FIGURE 4.10. Contour plot of $f_2$ for design 3.

FIGURE 4.11. Design 4. Density distribution of compliant material in L-shaped cross section optimized for torsional rigidity only.
FIGURE 4.12. Design 5. Density distribution of compliant material in L-shaped cross section optimized for torsional rigidity subject to rigidity with $p = 2$ integral penalty on $f_2$.

FIGURE 4.13. Contour plot of $f_2$ for design 4.

5. Plane Strain Problem with Layered Material

5.1 The Formulation of the Problem

In this chapter we want to consider two examples for linear elasticity with locally layered material. The first one is a flange with a L-shaped cross section. On one side the flange is fixed and on the other side a uniform load is applied over the length of the flange (see figure 5.1). As a second example we use a bar which is fixed at the sides and a traction load is applied at the bottom (see figure 5.2). Both are three dimensional problems which can be reduced to two dimensional plane strain problems (see chapter 2). Therefore the computations can be done for a cross section of the structures.

The characteristic length scale of the microgeometry is assumed to be small relative to the dimensions of the shaft cross section and is denoted by $\varepsilon$. In the neighborhood of any point $x = (x_1, x_2)$ the local microgeometry is given by layers of stiff material interspersed with layers of compliant material. The thickness of the stiff and compliant layers are specified by $\varepsilon \vartheta_1$ and $\varepsilon \vartheta_2$ respectively, with $\vartheta_1 + \vartheta_2 = 1$.

The layer normals are specified by the angle $\gamma$. The thickness of the layers and layering orientation is free to change across the cross section. The design variables are given by the thickness $\vartheta = \vartheta_1$ of the material one layer and the layer angle $\gamma$.

The mathematical formulation of the homogenized problem is the following: Given a domain $\Omega$ with boundary $\Gamma$. Compute the homogenized displacement $u$ which is the solution of

\[
\begin{cases}
-\text{div } \sigma = f & \text{in } \Omega \\
\sigma = C^E \varepsilon(u) & \text{in } \Omega \\
\sigma_n = g & \text{at } \Gamma_N \\
u = 0 & \text{at } \Gamma_D
\end{cases}
\]  

(5.1)

where

$$
\varepsilon(u) = \begin{pmatrix}
\frac{1}{2} \left( \frac{\partial u_1}{\partial x_1} \right) & \frac{1}{2} \left( \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1} \right) \\
\frac{1}{2} \left( \frac{\partial u_1}{\partial x_2} - \frac{\partial u_2}{\partial x_1} \right)
\end{pmatrix}
$$

(5.2)

is the strain tensor and $g$ is defined as shown in figures 5.1 and 5.2. The material property $C^E = C^E(\vartheta, \gamma)$ is the effective elasticity tensor of the layered material which is given by

$$
C^E = \vartheta A^1 \xi^1 + (1 - \vartheta) A^2 \xi^2
$$

(5.3)

where $A^1, A^2$ are the elastic tensors which map strains to stresses and $\xi^1, \xi^2$ are the strains in material one and two. The derivation of the explicit formulas for the elements of $C^E$ are given in chapter 6, see (6.307)-(6.318). For the computations we approximate the load as functions of type $g(y) = ae^{b(y-y_0)^2} - c$ for the first example and $g(x) = ae^{b(x-x_0)^2} - c$ for the second example. Here for example one $y_0$ is the $y$ coordinate and for example two $x_0$ is the $x$ coordinate of the center of the side where the load is applied and $a, b, c$ are parameters which can be chosen in an appropriate way.

In our context material one represents a reinforcement which means it is the stiffer material, so we have that $E_1 > E_2$. Usually there is not a big difference between the Poisson ratio of the reinforcement and the matrix material. Therefore we have chosen $\nu_1 = \nu_2$. From table 2.3 we obtain for the shear and bulk moduli of the two materials $\mu_1 > \mu_2$ and $\kappa_1 > \kappa_2$.

The work against the load is in general defined as the integral over all applied forces

$$
W(\vartheta, \gamma) = \int_{\Omega} f \cdot u \, dx + \int_{\Gamma_N} g \cdot u \, ds.
$$

(5.4)
For the homogenized cross sections we assume that there are no body forces so $f = 0$ and (5.4) simplifies to

$$W(\vartheta, \gamma) = \int_{\Gamma_N} g \cdot u \, ds. \quad (5.5)$$

The stress in the homogenized shaft is given by $\sigma = C^\varepsilon \varepsilon$. The macroscopic stress constraints associated with materials one and two are given in terms of the macrostress modulation functions introduced in [15]. The explicit formulas for material one and two are given by

$$f^1(\vartheta, \gamma) = Q^1(\vartheta, \gamma) \xi : \xi = |A^1 \xi|^2$$ \hspace{1cm} (5.6)

$$f^2(\vartheta, \gamma) = Q^2(\vartheta, \gamma) \xi : \xi = |A^2 \xi|^2$$ \hspace{1cm} (5.7)

for every $2 \times 2$ matrix $\xi$. The derivation of the elements of the stress amplification tensors $Q^1$ and $Q^2$ are given in chapter 6.

FIGURE 5.1. The domain $\Omega$ for the first example: a cross section of a flange.

The homogenized design problem is to minimize $W$ subject to a constraint on $f^i, i = 1, 2$ over a subset $S \subset \Omega$, i.e.,

$$\inf_{(\vartheta, \gamma)} \left\{ W(\vartheta, \gamma) \left| \int_{\Omega} f^i(\vartheta, \gamma) \, dx < K, \ 0 \leq \gamma \leq 2\pi, \ \int \vartheta_1 \, dx < \Theta |\Omega| \right. \right\}.$$ \hspace{1cm} (5.8)

FIGURE 5.2. The domain $\Omega$ for the second example: a cross section of a bar.
5.2 Identification of Graded Microstructure for Two Dimensional Elasticity

The procedure for identifying the discrete graded microgeometry for this problem follows the same steps outlined from the scalar problems presented in chapters 3 and 4. We state without proof the identification theorem for two dimensional elastic problem.

**Theorem 5.1.** Identification of graded microstructure for two dimensional elasticity.

For any given \( k > K \) and small number \( \delta > 0 \), one can construct a partition \( P_{\tau N_0} \) and locally layered microstructure specified by \( S_{\epsilon 0, N_0} \) for which the part of \( S \) over which the constraints

\[ \chi_1^{\epsilon 0, N_0}(x) | \sigma^{\epsilon 0, N_0}(x) | \leq t, \ i = 1, 2 \]  

(5.9)

are violated has measure (area) less than \( \delta \) and

\[ \left| \int_{\Omega} f \cdot u^{\epsilon 0, N_0} dx + \int_{\Gamma} g \cdot u^{\epsilon 0, N_0} ds - W(\hat{\theta}, \hat{\gamma}) \right| < \delta, \]  

(5.10)

and

\[ \int_{\Omega} \chi_1^{\epsilon 0, N_0} dx_1 dx_2 \leq \Theta \times (\text{Area of } \Omega \)+ \delta. \]  

(5.11)

Inside each subdomain \( \omega^k \) associated with the partition \( P_{\tau N_0} \) the local layer directions and area fractions are determined from the optimal homogenized design \((\hat{\theta}_1, \hat{\gamma})\) through the averages given by

\[ \hat{\theta}_1^k = \frac{1}{\text{Area of } \omega^k} \times \int_{\omega^k} \hat{\theta}_1(x) dx_1 dx_2, \]  

(5.12)

\[ \hat{\gamma}^k = \frac{1}{\text{Area of } \omega^k} \times \int_{\omega^k} \hat{\gamma}(x) dx_1 dx_2. \]  

(5.13)

5.3 Computational Approach to the Homogenized Design Problem

In this section we show how to obtain updates for the design variables using a gradient algorithm.

Define the space \( V_0 \) as follows

\[ V_0 = \{ u \in H^1(\Omega)^2, \ u = 0 \text{ on } \Gamma_D \}. \]  

(5.14)

In the given problem (5.1) we perturb \( \theta \) and \( \gamma \) by \( \hat{\theta} \) and \( \hat{\gamma} \) we obtain a perturbed solution \( u + \hat{u} \)

\[ -\text{div} \left( C^E(\theta + \hat{\theta}, \gamma + \hat{\gamma}) \epsilon(u + \hat{u}) \right) = f \text{ in } \Omega \]  

\[ C^E(\theta + \hat{\theta}, \gamma + \hat{\gamma}) \epsilon(u + \hat{u}) n = g \text{ on } \Gamma_N. \]  

(5.15)

Replacing \( C^E(\theta + \hat{\theta}, \gamma + \hat{\gamma}) \) by its Taylor series stopped after the linear term

\[ C^E(\theta + \hat{\theta}, \gamma + \hat{\gamma}) = C^E(\theta, \gamma) + \partial_\theta C^E(\theta, \gamma) \hat{\theta} + \partial_\gamma C^E(\theta, \gamma) \hat{\gamma} + o(\hat{\theta}^2, \hat{\gamma}^2) \]  

(5.16)

and neglecting the remainder term we obtain for (5.15)

\[ -\text{div} \left( \left( C^E(\theta, \gamma) + \partial_\theta C^E(\theta, \gamma) \hat{\theta} + \partial_\gamma C^E(\theta, \gamma) \hat{\gamma} \right) \epsilon(u + \hat{u}) \right) = f \text{ in } \Omega \]  

\[ C^E(\theta, \gamma) + \partial_\theta C^E(\theta, \gamma) \hat{\theta} + \partial_\gamma C^E(\theta, \gamma) \hat{\gamma} \epsilon(u + \hat{u}) n = g \text{ on } \Gamma_N. \]  

(5.17)
Expanding the equations and collecting only first order perturbation terms we have

\[-\text{div} \left( C^E(\vartheta, \gamma)\epsilon(u) + \left( \partial_\vartheta C^E(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma C^E(\vartheta, \gamma) \hat{\gamma} \right) \epsilon(u) + C^E(\vartheta, \gamma)\epsilon(\hat{u}) \right) = f \quad \text{in } \Omega \]

\[
\left( C^E(\vartheta, \gamma)\epsilon(u) + \left( \partial_\vartheta C^E(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma C^E(\vartheta, \gamma) \hat{\gamma} \right) \epsilon(u) + C^E(\vartheta, \gamma)\epsilon(\hat{u}) \right) n = g \quad \text{on } \Gamma_N. \tag{5.18}
\]

Subtracting equations (5.1) from (5.18) it remains

\[
-\text{div} \left( C^E(\vartheta, \gamma)\epsilon(\hat{u}) \right) = \text{div} \left( \left( \partial_\vartheta C^E(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma C^E(\vartheta, \gamma) \hat{\gamma} \right) \epsilon(u) \right) \quad \text{in } \Omega \\
C^E(\vartheta, \gamma)\epsilon(\hat{u}) n = - \left( \partial_\vartheta C^E(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma C^E(\vartheta, \gamma) \hat{\gamma} \right) \epsilon(u) n \quad \text{on } \Gamma_N. \tag{5.19}
\]

In weak formulation we have for all \(w \in V_0\)

\[
\int_\Omega C^E(\vartheta, \gamma)\epsilon(\hat{u}) (w) \, dx = -\int_\Omega \left( \partial_\vartheta C^E(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma C^E(\vartheta, \gamma) \hat{\gamma} \right) \epsilon(u) (w) \, dx. \tag{5.20}
\]

The homogenized design problem (5.8) can be expressed as minimizing the linear functional \(L = L(\vartheta, \gamma)\) where \(L\) is given by

\[
L = \int_\Omega f \cdot u \, dx + \int_{\Gamma_N} g \cdot u \, ds + l_1 \int_\Omega \vartheta \, dx + l_2 \int_\Omega Q^i(\vartheta, \gamma)\epsilon(u) : \epsilon(u) \, dx. \tag{5.21}
\]

For a perturbed solution \(u + \hat{u}\) the functional becomes

\[
L + \hat{L} = \int_\Omega f (u + \hat{u}) \, dx + \int_{\Gamma_N} g (u + \hat{u}) \, ds + l_1 \int_\Omega (\vartheta + \hat{\vartheta}) \, dx + l_2 \int_\Omega Q^i(\vartheta + \hat{\vartheta}, \gamma + \hat{\gamma})\epsilon(u + \hat{u}) : \epsilon(u + \hat{u}) \, dx. \tag{5.22}
\]

Replacing \(Q^i(\vartheta + \hat{\vartheta}, \gamma + \hat{\gamma})\) by its Taylor series stopped after the linear term

\[
Q^i(\vartheta + \hat{\vartheta}, \gamma + \hat{\gamma}) = Q^i(\vartheta, \gamma) + \partial_\vartheta Q^i(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma Q^i(\vartheta, \gamma) \hat{\gamma} + o(\hat{\vartheta}^2, \hat{\gamma}^2) \tag{5.23}
\]

and neglecting the remainder term we obtain for (5.22)

\[
L + \hat{L} = \int_\Omega f \cdot (u + \hat{u}) \, dx + \int_{\Gamma_N} g \cdot (u + \hat{u}) \, ds + l_1 \int_\Omega (\vartheta + \hat{\vartheta}) \, dx + \\
+ l_2 \int_\Omega \left[ 2Q^i(\vartheta, \gamma)\epsilon(u) : \epsilon(u) + (\partial_\vartheta Q^i(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma Q^i(\vartheta, \gamma) \hat{\gamma})\epsilon(u) : \epsilon(u) \right] \, dx. \tag{5.24}
\]

For the change of \(L\) we collect only first order perturbation terms

\[
\hat{L} = \int_\Omega f \cdot \hat{u} \, dx + \int_{\Gamma_N} g \cdot \hat{u} \, ds + l_1 \int_\Omega \hat{\vartheta} \, dx + \\
l_2 \int_\Omega \left[ 2Q^i(\vartheta, \gamma)\epsilon(u) : \epsilon(u) + (\partial_\vartheta Q^i(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma Q^i(\vartheta, \gamma) \hat{\gamma})\epsilon(u) : \epsilon(u) \right] \, dx. \tag{5.25}
\]

We introduce the adjoint field \(v \in V_0\) where \(v\) is the solution of

\[-\text{div} \left( C^E(\vartheta, \gamma)\epsilon(v) \right) = f - l_2 \text{div} \left( 2Q^i(\vartheta, \gamma)\epsilon(u) \right) \quad \text{in } \Omega \]

\[
C^E(\vartheta, \gamma)\epsilon(v) n = g + 2Q^i(\vartheta, \gamma)\epsilon(u) n \quad \text{on } \Gamma_N. \tag{5.26}
\]

In weak formulation we have

\[
\int_\Omega C^E(\vartheta, \gamma)\epsilon(v) : \epsilon(w) \, dx - \int_{\Gamma_N} g \cdot w \, ds - \int_{\Gamma_N} 2Q^i(\vartheta, \gamma)\epsilon(u) n \cdot w \, ds = \\
\int_\Omega f \cdot w \, dx + l_2 \int_{\Gamma_N} 2Q^i(\vartheta, \gamma)\epsilon(v) : \epsilon(w) \, dx - \int_{\Gamma_N} 2Q^i(\vartheta, \gamma)\epsilon(u) n \cdot w \, ds. \tag{5.27}
\]
or
\[
\int_\Omega C^E(\vartheta, \gamma) \epsilon(v) : \epsilon(w) \, dx = \int_{\Gamma_N} g \cdot w \, ds + \int_\Omega f \cdot w \, dx + l_2 \int_\Omega 2Q^i(\vartheta, \gamma) \epsilon(u) : \epsilon(w) \, dx \quad (5.28)
\]
for all \( w \in V_0 \). For \( w = \hat{u} \) we obtain
\[
\int_\Omega C^E(\vartheta, \gamma) \epsilon(v) : \epsilon(\hat{u}) \, dx = \int_{\Gamma_N} g \cdot \hat{u} \, ds + \int_\Omega f \cdot \hat{u} \, dx + l_2 \int_\Omega 2Q^i(\vartheta, \gamma) \epsilon(u) : \epsilon(\hat{u}) \, dx. \quad (5.29)
\]
Combining (5.20) and (5.29) we have
\[
\int_{\Gamma_N} g \cdot \hat{u} \, ds + \int_\Omega f \cdot \hat{u} \, dx + l_2 \int_\Omega 2Q^i(\vartheta, \gamma) \epsilon(u) : \epsilon(\hat{u}) \, dx = - \int_\Omega \left( \partial_\vartheta C^E(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma C^E(\vartheta, \gamma) \right) \epsilon(u) : \epsilon(v) \, dx. \quad (5.30)
\]
Now we can continue with (5.25) to obtain
\[
\hat{L} = - \int_\Omega \left( \partial_\vartheta C^E(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma C^E(\vartheta, \gamma) \right) \epsilon(u) : \epsilon(v) \, dx + l_1 \int_\Omega \hat{\vartheta} \, dx + l_2 \int_\Omega \left( \partial_\vartheta Q^i(\vartheta, \gamma) \hat{\vartheta} + \partial_\gamma Q^i(\vartheta, \gamma) \hat{\gamma} \right) \epsilon(u) : \epsilon(u) \, dx. \quad (5.31)
\]
The choice of \( \hat{\vartheta} \) and \( \hat{\gamma} \) that renders \( \delta L \) the most negative is given by
\[
\hat{\vartheta} = \partial_\vartheta C^E(\vartheta, \gamma) \epsilon(u) : \epsilon(v) - l_1 - l_2 \partial_\vartheta Q^i(\vartheta, \gamma) \epsilon(u) : \epsilon(u) \quad (5.32)
\]
\[
\hat{\gamma} = \partial_\gamma C^E(\vartheta, \gamma) \epsilon(u) : \epsilon(v) - l_2 \partial_\gamma Q^i(\vartheta, \gamma) \epsilon(u) : \epsilon(u). \quad (5.33)
\]
The updated design variables are obtained by
\[
\vartheta_{i+1} = \vartheta_i + \varepsilon_\vartheta \hat{\vartheta} \quad (5.33)
\]
\[
\gamma_{i+1} = \gamma_i + \varepsilon_\gamma \hat{\gamma} \quad (5.34)
\]
where \( \varepsilon_\vartheta \) and \( \varepsilon_\gamma \) are parameters which give control how far to step in the optimal direction.

### 5.4 The Results
The computations were done using the finite element method with a triangular mesh and linear shape function for the L-shaped cross section. The Poisson’s ratio for both materials is \( \nu_1 = \nu_2 = 0.3 \). The Young’s modulus of the stiff material is ten times greater than the one of the compliant material. In all cases the volume fraction of the reinforcement is 30%. The first design is just a homogeneous material. The design (see figure 5.3) which is optimized for work against the load shows a clear drop in this quantity, while the stresses are about the same as for the homogeneous material. The third design (see figure 5.4) has lower stresses than designs 1 and 2 but the work against the load is high. The fourth design (see 5.5) is a mixture of 2 and 3. It shows reasonable stresses and the work against the load remains small. One can see the tendency to take stiff material out of the corner to minimize the local stresses.

For the second example the concentration of the reinforcement is 40%. The figures are produced using the finite element method with a rectangular mesh and linear shape functions. Figure 5.7 shows a design which is optimized for work against the load. The layer direction is vertical. In figure 5.8 the design is optimized for stresses. Here the layer direction of the reinforcement is horizontal. In both cases the layer direction does not change during the optimization process.

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TABLE 5.1. Work against the load and stresses for the different designs.

<table>
<thead>
<tr>
<th>Design #</th>
<th>optimized for</th>
<th>Vol. Fraction</th>
<th>Work against load</th>
<th>Stress Integral</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>nothing</td>
<td>30%</td>
<td>5.347930</td>
<td>34228.791675</td>
</tr>
<tr>
<td>2</td>
<td>work against load</td>
<td>30%</td>
<td>2.064640</td>
<td>35309.747031</td>
</tr>
<tr>
<td>3</td>
<td>stress</td>
<td>30%</td>
<td>7.005334</td>
<td>20972.733988</td>
</tr>
<tr>
<td>4</td>
<td>work against load and stress</td>
<td>30%</td>
<td>2.629880</td>
<td>28931.904073</td>
</tr>
</tbody>
</table>

FIGURE 5.3. Design optimized for work against the load.
FIGURE 5.4. Design optimized for stress.

FIGURE 5.5. Design optimized for work against the load and stress.
FIGURE 5.6. Stresses for the four cases.

A. Homogeneous material.  
B. Work against load optimized.  
C. Stress optimized.  
D. Work against load and stress optimized.
FIGURE 5.7. Design optimized for work against the load.

FIGURE 5.8. Design optimized for stress.
6. Derivations for the Plane Strain Problem

6.1 Derivation of the Material Property Tensors

In this section we derive explicit formulas for the effective stiffness tensor and the stress amplification tensor. For this discussion we consider two-phase layered materials. Here the two components are referred to as material one and material two. The thickness of the layers is given by \( \vartheta_1 \) and \( \vartheta_2 \) with \( \vartheta_1 + \vartheta_2 = 1 \) and the layer normal by \( n = (n_1 \ n_2)^T \).

Given an applied constant strain \( \bar{\xi} = (\bar{\xi}_{11} \ \bar{\xi}_{12} \ \bar{\xi}_{21} \ \bar{\xi}_{22}) \).

The strain tensor is symmetric so \( \bar{\xi}_{12} = \bar{\xi}_{21} \). The elastic property of material one is \( A_1 \) and of material two is \( A_2 \). The elastic tensors \( A_1 \) and \( A_2 \) map strains to stresses. In this context \( A_1 \) and \( A_2 \) represent isotropic elastic materials characterized by bulk and shear moduli \( (\kappa_1, \mu_1) \) and \( (\kappa_2, \mu_2) \) (see section 2.1).

Now we want to define the elastic properties. Given a strain \( \epsilon = (\epsilon_{11} \ \epsilon_{12} \ \epsilon_{21} \ \epsilon_{22}) \)

we have that

\[
A_i \epsilon = 2\mu_i(\epsilon - \frac{1}{2}\text{tr}\epsilon) + 2\kappa_i\frac{1}{2}\text{tr}\epsilon, \quad i = 1, 2
\]

with \( \text{tr}\epsilon = \epsilon_{11} + \epsilon_{22} \) and \( I \) is the two dimensional identity matrix. The matrix

\[
\epsilon - \frac{1}{2}\text{tr}\epsilon I = \epsilon^D
\]

is called the deviatoric part of the strain \( \epsilon \) and the matrix

\[
\frac{1}{2}\text{tr}\epsilon I = \epsilon^H
\]

is called the spherical or hydrostatic part of \( \epsilon \). So we can write (6.3) as

\[
A_i \epsilon = 2\mu_i\epsilon^D + 2\kappa_i\epsilon^H, \quad i = 1, 2.
\]

The elastic problem in the unit cell \( Q = \{(x_1, x_2) | (x_1, x_2) \in (0, 1) \times (0, 1)\} \) is given by: Solve

\[
\text{div}(A_i(\tilde{\epsilon} + \bar{\xi})) = 0, \quad i = 1, 2
\]

in material \( i \) where

\[
\tilde{\epsilon} = \begin{pmatrix}
\frac{\partial x_1 w_1}{2} & \frac{\partial x_1 w_2 + \partial x_2 w_1}{2} \\
\frac{\partial x_2 w_2 + \partial x_2 w_1}{2} & \partial x_2 w_2
\end{pmatrix}
\]

is the fluctuating strain and \( w = (w_1 \ w_2)^T \) is the \( Q \) periodic fluctuating displacement. On the interface between the two materials we have the two conditions

\[
A_1(\tilde{\epsilon} + \bar{\xi})n|_1 = A_2(\tilde{\epsilon} + \bar{\xi})n|_2
\]

which is the balance of forces and

\[
w|_1 = w|_2
\]
the continuity of displacements. The left hand sides of the two above equations describe the properties in material one and the right hand sides in material two. Since we have a layered geometry we suppose the strain is piecewise constant and so there is a constant strain inside each layer

\[
\tilde{\epsilon} + \xi = \bar{\xi}^i = \begin{pmatrix}
\tilde{\epsilon}_{11}^i & \tilde{\epsilon}_{12}^i \\
\tilde{\epsilon}_{21}^i & \tilde{\epsilon}_{22}^i 
\end{pmatrix}, \quad i = 1, 2.
\] (6.11)

With this assumption (6.7) becomes \( \text{div}(A^i \bar{\xi}) = 0, \quad i = 1, 2 \). Now we just have to choose \( \bar{\xi}^1 \) and \( \bar{\xi}^2 \) such that (6.9) and (6.10) are satisfied. From (6.11) we obtain

\[ w \text{ is a linear function in each of the layers.} \]

Because of this condition (6.10) can be written as

\[
\bar{\xi}_{ij}^1 - \bar{\xi}_{ij}^2 = \frac{n_i \lambda_j + n_j \lambda_i}{2} =: \lambda \odot n
\] (6.12)

where \( n = (n_1 \ n_2)^T \) is the layer normal and the vector \( \lambda = (\lambda_1 \ \lambda_2)^T \) is to be determined.

Last we observe that \( \bar{\xi} = \int_Q \epsilon \, dx \) where

\[
\epsilon(x) = \begin{cases}
\bar{\xi}_1 & \text{in layer 1} \\
\bar{\xi}_2 & \text{in layer 2}
\end{cases}
\] (6.13)

to get \( \bar{\xi} = \vartheta_1 \bar{\xi}_1 + \vartheta_2 \bar{\xi}_2 \).

So we have the system of 3 equations

\[
\vartheta_1 \bar{\xi}_1 + \vartheta_2 \bar{\xi}_2 = \bar{\xi}
\] (6.14)

\[
(A^1 \bar{\xi}_1)n = (A^2 \bar{\xi}_2)n
\] (6.15)

\[
\bar{\xi}_1 - \bar{\xi}_2 = \lambda \odot n
\] (6.16)

in the 3 matrix unknowns \( \bar{\xi}_1, \bar{\xi}_2 \) and \( \lambda \odot \). Also recall that \( \vartheta_1 + \vartheta_2 = 1 \).

To find the solution of \( \bar{\xi}_1, \bar{\xi}_2 \) and \( \lambda \) we start writing \( \bar{\xi}_1 \) in terms of \( \bar{\xi} \) using (6.14)

\[
\bar{\xi}_1 = \vartheta_1^{-1}(\bar{\xi} - \vartheta_2 \bar{\xi}_2).
\] (6.17)

Next we eliminate \( \bar{\xi}_1 \) from (6.16) to obtain

\[
\bar{\xi}_2 = \bar{\xi} - \vartheta_1 \lambda \odot n.
\] (6.18)

Now solve for \( \bar{\xi}_1 \) in terms of \( \bar{\xi} \) and \( \lambda \odot n \) using (6.17) and (6.18)

\[
\bar{\xi}_1 = \bar{\xi} + \vartheta_2 \lambda \odot n.
\] (6.19)

Next we obtain explicit formulas for \( \bar{\xi}_1 \) and \( \bar{\xi}_2 \) in terms of layer direction \( n \) and volume fraction \( \vartheta_1 \) and \( \vartheta_2 \). To do this we start by getting a formula for \( \lambda \odot n \). For this we substitute (6.18) and (6.19) into (6.15)

\[
A^1(\bar{\xi} + \vartheta_2 \lambda \odot n)n = A^2(\bar{\xi} - \vartheta_1 \lambda \odot n)n.
\] (6.20)

Computing the left side of (6.20) we obtain

\[
A^1 \bar{\xi} = 2\mu_1(\bar{\xi} - \frac{\text{tr} \bar{\xi}}{2} I) + 2\kappa_1 \frac{\text{tr} \bar{\xi}}{2} I
\] (6.21)

\[
A^1(\lambda \odot n) = 2\mu_1(\lambda \odot n - \frac{\text{tr}(\lambda \odot n)}{2} I) + 2\kappa_1 \frac{\text{tr}(\lambda \odot n)}{2} I.
\] (6.22)
With $\text{tr}(\lambda \odot n) = \lambda \cdot n$ we have

$$A^1(\tilde{\xi} + \vartheta_2(\lambda \odot n)) = 2\mu_1(\tilde{\xi} - \frac{\text{tr} \xi}{2} I) + 2\kappa_1 \frac{\text{tr} \xi}{2} I + \vartheta_2(2\mu_1(\lambda \odot n - \frac{\lambda n}{2} I) + 2\kappa_1 \frac{\lambda n}{2} I) \quad (6.23)$$

and analogously

$$A^2(\tilde{\xi} - \vartheta_1(\lambda \odot n)) = 2\mu_2(\tilde{\xi} - \frac{\text{tr} \xi}{2} I) + 2\kappa_2 \frac{\text{tr} \xi}{2} I + \vartheta_2(2\mu_2(\lambda \odot n - \frac{\lambda n}{2} I) + 2\kappa_2 \frac{\lambda n}{2} I). \quad (6.24)$$

Note that

$$(\lambda \odot n)_{ij} n_j = \frac{1}{2}(\lambda_i n_j + \lambda_j n_i) = \frac{1}{2}(\lambda + (\lambda \cdot n)n). \quad (6.25)$$

Using (6.25) we finally obtain for both sides of (6.20)

$$A^1(\tilde{\xi} + \vartheta_2(\lambda \odot n)) n = 2\mu_1(\tilde{\xi} n - \frac{\text{tr} \xi}{2} n) + 2\kappa_1 \frac{\text{tr} \xi}{2} n + \vartheta_2(2\mu_1 \frac{\lambda}{2} + 2\kappa_1 \frac{\lambda n}{2} n) \quad (6.26)$$

$$A^2(\tilde{\xi} - \vartheta_1(\lambda \odot n)) n = 2\mu_2(\tilde{\xi} n - \frac{\text{tr} \xi}{2} n) + 2\kappa_2 \frac{\text{tr} \xi}{2} n - \vartheta_1(2\mu_2 \frac{\lambda}{2} + 2\kappa_1 \frac{\lambda n}{2} n) \quad (6.27)$$

Now we will first solve for $\lambda \cdot n$ by multiplying (6.15) by $n$

$$(A^1 \tilde{\xi}n) \cdot n = (A^2 \tilde{\xi}n) \cdot n \quad (6.28)$$

and substitute in (6.26) and (6.27) to get

$$2\mu_1(\tilde{\xi} n - \frac{\text{tr} \xi}{2} n) + 2\kappa_1 \frac{\text{tr} \xi}{2} + \vartheta_2(2\mu_1 \frac{\lambda n}{2} + 2\kappa_1 \frac{\lambda n}{2} n) = 2\mu_2(\tilde{\xi} n - \frac{\text{tr} \xi}{2} n) + 2\kappa_2 \frac{\text{tr} \xi}{2} - \vartheta_1(2\mu_1 \frac{\lambda}{2} + 2\kappa_1 \frac{\lambda n}{2}) \quad (6.29)$$

Solving for $\lambda \cdot n$ gives

$$\lambda \cdot n = \frac{\Delta \mu(2\tilde{\xi} n - \text{tr} \xi) + \Delta \kappa \text{tr} \xi}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \quad (6.30)$$

where

$$\Delta \mu = \mu_2 - \mu_1 \quad (6.31)$$

$$\Delta \kappa = \kappa_2 - \kappa_1 \quad (6.32)$$

$$\langle \bar{\mu} \rangle = \vartheta_2 \mu_1 + \vartheta_1 \mu_2 \quad (6.33)$$

$$\langle \bar{\kappa} \rangle = \vartheta_2 \kappa_1 + \vartheta_1 \kappa_2. \quad (6.34)$$

Now we use (6.15) and solve for $\lambda$. So from (6.26) and (6.27) we get

$$2\mu_1(\tilde{\xi} n - \frac{\text{tr} \xi}{2} n) + \kappa_1 \text{tr} \xi n + \vartheta_2(\mu_1 \lambda + \kappa_1 \lambda n) = 2\mu_2(\tilde{\xi} n - \frac{\text{tr} \xi}{2} n) + \kappa_2 \text{tr} \xi n - \vartheta_1(\mu_1 \lambda + \kappa_1 \lambda n) \quad (6.35)$$

$$2\Delta \mu(\tilde{\xi} n - \frac{\text{tr} \xi}{2} n) + 2\Delta \kappa \text{tr} \xi n = \langle \bar{\mu} \rangle \lambda + \langle \bar{\kappa} \rangle (\lambda \cdot n) \quad (6.36)$$

and

$$\lambda = \frac{\Delta \mu}{\langle \bar{\mu} \rangle}(2\xi n - \text{tr} \xi n) + \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} \text{tr} \xi n - \langle \bar{\kappa} \rangle \langle \bar{\mu} \rangle (\lambda \cdot n) \quad (6.37)$$

Substituting (6.30) leads to

$$\lambda = \frac{\Delta \mu}{\langle \bar{\mu} \rangle}(2\xi n - \text{tr} \xi n) + \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} \text{tr} \xi n - \langle \bar{\kappa} \rangle \left( \frac{\Delta \mu(2\xi n - \text{tr} \xi) + \Delta \kappa \text{tr} \xi}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) n. \quad (6.38)$$

For $\lambda \odot n$ we find

$$\lambda \odot n = \frac{\Delta \mu}{\langle \bar{\mu} \rangle}(2(\xi n) \odot n - \text{tr} \xi n \odot n) + \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} \text{tr} \xi n \odot n - \langle \bar{\kappa} \rangle \left( \frac{\Delta \mu(2\xi n \cdot n - \text{tr} \xi) + \Delta \kappa \text{tr} \xi}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) n \odot n. \quad (6.39)$$
We conclude by noting that the strains in material one and two are given by (6.18) and (6.19) together with (6.39).

We now develop explicit formulas for the elements of the effective elastic tensor for layered materials \( C^E \) where

\[
C^E = \vartheta_1 A^1 \xi^1 + \vartheta_2 A^2 \xi^2
\]

and \( \xi^1, \xi^2 \) are given by (6.18) and (6.19) as well as the tensors \( Q^1 \) and \( Q^2 \) given by

\[
Q^1 \xi : \bar{\xi} = |A^1 \xi^1|^2
\]
\[
Q^2 \xi : \bar{\xi} = |A^2 \xi^2|^2.
\]

We can express the normal vector \( n \) as \( n = (\cos \gamma \ sin \gamma)^T \) where \( \gamma \) is the layer angle. So we can write explicit formulas for the constant strain fields \( \bar{\xi}_1 \) and \( \bar{\xi}_2 \) in terms of layer angle and layer thickness.

Next we want to express the properties in terms of a basis of \( \mathbb{R}^2 \). For \( \lambda \cdot n \) we have using (6.30)

\[
\lambda \cdot n = \frac{2\Delta \mu \left( \begin{array}{c}
\bar{\xi}_{11} \\
\bar{\xi}_{21}
\end{array} \right) \left( \begin{array}{c}
n_1 \\
n_2
\end{array} \right) \cdot \left( \begin{array}{c}
n_1 \\
n_2
\end{array} \right) - \Delta \mu (\bar{\xi}_{11} + \bar{\xi}_{22}) + \Delta \kappa (\bar{\xi}_{11} + \bar{\xi}_{22})}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \tag{6.43}
\]

and for \( \lambda \) using (6.38)

\[
\lambda = \frac{\Delta \mu}{\langle \bar{\mu} \rangle} \left( \begin{array}{c}
\bar{\xi}_{11}n_1 + 2\bar{\xi}_{12}n_2 - \bar{\xi}_{22}n_1 \\
2\bar{\xi}_{21}n_1 + \bar{\xi}_{22}n_2 - \bar{\xi}_{11}n_2
\end{array} \right) + \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} \left( \begin{array}{c}
\bar{\xi}_{11}n_1 + \bar{\xi}_{22}n_1 \\
\bar{\xi}_{11}n_2 + \bar{\xi}_{22}n_2
\end{array} \right) - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \lambda_n \left( \begin{array}{c}
n_1 \\
n_2
\end{array} \right). \tag{6.47}
\]

So we obtain for \( \lambda_1 \)

\[
\lambda_1 = \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) n_1 \bar{\xi}_{11} + \frac{2n_2^2 \Delta \mu - \langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2n_2 \Delta \mu}{\langle \bar{\mu} \rangle} \frac{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle}{n_1} \bar{\xi}_{12} \tag{6.48}
\]

and for \( \lambda_2 \)

\[
\lambda_2 = \left( \frac{\Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) n_2 \bar{\xi}_{11} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2n_1 \Delta \mu}{\langle \bar{\mu} \rangle} \frac{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle}{n_2} \bar{\xi}_{12} \tag{6.50}
\]

To obtain \( \lambda \odot n \) using (6.25) we first compute \( (\bar{\xi}_n) \odot n \)

\[
(\bar{\xi}_n) \odot n = \left( \begin{array}{c}
\xi_{11}n_1 + \xi_{12}n_2 \\
\xi_{21}n_1 + \xi_{22}n_2
\end{array} \right) \odot \left( \begin{array}{c}
n_1 \\
n_2
\end{array} \right) \tag{6.52}
\]

\[
= \left( \begin{array}{c}
\frac{1}{2} (n_1^2 \xi_{11} + n_1^2 \xi_{12} + n_2^2 \xi_{11} + n_2^2 \xi_{12} + n_1 n_2 \xi_{11} + n_1 n_2 \xi_{12}) \\
\frac{1}{2} (n_1^2 \xi_{21} + n_1^2 \xi_{22} + n_2^2 \xi_{21} + n_2^2 \xi_{22} + n_1 n_2 \xi_{21} + n_1 n_2 \xi_{22})
\end{array} \right) \tag{6.53}
\]
then compute $\text{tr} \xi n \odot n$

$$\text{tr} \xi n \odot n = \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) n_1^2 \xi_{11}$$

$$= \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{\Delta \mu}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) n_1^2 n_2 \xi_{12} + \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} n_1^2 \xi_{21}$$

$$+ \left( \frac{n_2^2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{n_1^2 n_2}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) \bar{\xi}_{11}$$

$$+ \left( \frac{n_2^2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{n_1^2 n_2}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) \bar{\xi}_{21}$$

$$+ \left( \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) n_1 n_2 \bar{\xi}_{22}$$

$$= \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{\Delta \mu}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \right) n_1 n_2 \bar{\xi}_{22}.$$
\[ + \left( \frac{\Delta \mu}{\langle \tilde{\mu} \rangle} - \frac{\langle \kappa \rangle}{\langle \tilde{\mu} \rangle} \frac{\Delta \mu}{\langle \tilde{\mu} \rangle + \langle \kappa \rangle} \right) 2n_1n_2 \tilde{\xi}_{21} \]
\[ + \left( \frac{\Delta \mu + \Delta \kappa}{\langle \tilde{\mu} \rangle} - \frac{\langle \kappa \rangle}{\langle \tilde{\mu} \rangle} \frac{2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \kappa \rangle} \right) n_2^2 \tilde{\xi}_{22}. \]

The constant strain field in layer one is \( \tilde{\xi}_1 \) given by
\[ \tilde{\xi}_1 = \tilde{\xi} + \vartheta_2 \lambda \odot n. \] (6.73)

The constant strain field in layer two is \( \tilde{\xi}_2 \) given by
\[ \tilde{\xi}_2 = \tilde{\xi} - \vartheta_1 \lambda \odot n. \] (6.74)

Compute \( C^i \tilde{\xi} \), \( i = 1, 2 \)
\[ C^1 \tilde{\xi} = A^1 \tilde{\xi} = A^1 \tilde{\xi} + \vartheta_2 A^1(\lambda \odot n) \] (6.75)
\[ C^2 \tilde{\xi} = A^2 \tilde{\xi} - \vartheta_1 A^2(\lambda \odot n) \] (6.76)

where \( A^i \tilde{\xi} \) is given by
\[ A^i \tilde{\xi} = 2 \mu_i \left( \tilde{\xi} - \frac{1}{4} \text{tr} I + 2 \kappa \frac{1}{2} \text{tr} \tilde{I} \right) + 2 \kappa \frac{1}{2} \text{tr} \tilde{I} \] (6.78)
\[ = \left( \frac{\mu_i \tilde{\xi}_{11} - \mu_i \tilde{\xi}_{22}}{2 \mu_i \tilde{\xi}_{21}} \right) + \left( \frac{\kappa \tilde{\xi}_{11} + \kappa \tilde{\xi}_{22}}{0 \kappa \tilde{\xi}_{11} + \kappa \tilde{\xi}_{22}} \right) \] (6.79)
\[ = \left( \frac{(\mu_i + \kappa) \tilde{\xi}_{11} + (\kappa - \mu_i) \tilde{\xi}_{22}}{2 \mu_i \tilde{\xi}_{21}} \right) + \left( \kappa - \mu_i \tilde{\xi}_{11} + \mu_i + \kappa \tilde{\xi}_{22} \right) \] (6.80)

and \( A^i(\lambda \odot n) \) is given by
\[ A^i(\lambda \odot n) = 2 \mu_i \left( \lambda \odot n - \frac{1}{2} \text{tr} (\lambda \odot n) I \right) + 2 \kappa \frac{1}{2} \text{tr} (\lambda \odot n) I \] (6.81)
\[ A^i(\lambda \odot n) = 2 \mu_i \left( \lambda \odot n - \frac{1}{2} \text{tr} \lambda \odot n I \right) + 2 \kappa \frac{1}{2} \text{tr} \lambda \odot n I. \] (6.82)

Written differently we get
\[ A^i(\lambda \odot n) = 2 \mu_i \lambda \odot n + (\kappa_i - \mu_i) \text{tr} (\lambda \odot n) I. \] (6.83)

For the four components of \( A^i(\lambda \odot n) \) we obtain
\[ (A^i(\lambda \odot n))_{11} = 2 \mu_i (\lambda \odot n)_{11} + (\kappa_i - \mu_i) \left[ (\lambda \odot n)_{11} + (\lambda \odot n)_{22} \right] \] (6.84)
\[ = (\mu_i + \kappa_i)(\lambda \odot n)_{11} + (\kappa_i - \mu_i)(\lambda \odot n)_{22} \] (6.85)
\[ = \left( \frac{\Delta \mu + \Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_1 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_1^2 + \] (6.86)
\[ + \left( \frac{\Delta \kappa - \Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_2^2 \tilde{\xi}_{11} \] (6.87)
\[ + 2n_1 n_2 \left[ \frac{\kappa_i - \mu_i}{\langle \mu \rangle} \frac{\Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right] n_2^2 \tilde{\xi}_{12} \] (6.88)
\[ + \left( \frac{\kappa_i - \mu_i}{\langle \mu \rangle} \frac{\Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_2^2 \tilde{\xi}_{12} \] (6.89)
Now we can compute the four components of $C^1\tilde{\xi}$

$$C^1\tilde{\xi} = (A^1\tilde{\xi})_{11} + \varphi_2 (A^1(\lambda \circ n))_{11}$$

$$= \left[ (\mu_1 + \lambda) + \varphi_2 (\mu_1 + \lambda) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\Delta \mu}{\langle \mu \rangle} \right) \right] n_1 + \varphi_1 (\lambda - \mu_1) \left( \Delta \kappa - \mu_1 \right) \left( \Delta \mu - \Delta \kappa - \Delta \mu \right) n_2^2$$

$$= (A^1(\lambda \circ n))_{12} = 2\mu_1(\lambda \circ n)_{12} + (\kappa_1 - \mu_1) [(\lambda \circ n)_{11} + (\lambda \circ n)_{22}]$$

$$= (\kappa_1 - \mu_1)[(\lambda \circ n)_{22} + (\kappa_1 - \mu_1) [(\lambda \circ n)_{21} + (\kappa_1 - \mu_1) [(\lambda \circ n)_{21} +$$

$$\left[ (\mu_1 + \lambda) - \frac{\Delta \mu}{\langle \bar{\mu} \rangle} \right] n_1 + \varphi_1 (\lambda - \mu_1) \left( \Delta \kappa - \mu_1 \right) \left( \Delta \mu - \Delta \kappa - \Delta \mu \right) n_2^2$$

Now we can compute the four components of $C^1\tilde{\xi}$
\[
+ \vartheta_2 2 n_1 n_2 \left[ - (\mu_1 + \kappa_1) \left( \frac{\Delta \mu}{\langle \mu \rangle} \right) \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1^2 + (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_2^2 \right] \xi_{21}
\]

\[
+ \left[ (\kappa_1 - \mu_1) + \vartheta_2 (\mu_1 + \kappa_1) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_2^2 \right] \xi_{22}
\]

\[
(C^1 \xi)_{12} = (A^1 \xi)_{12} + \vartheta_2 (A^1 (\lambda \otimes n))_{12}
\]

\[
= 2 \mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1 n_2 \xi_{11}
\]

\[
+ \left( 2 \mu_1 + 2 \mu_1 \vartheta_2 \frac{n_2^2 \Delta \mu}{\langle \mu \rangle} - 2 \mu_1 \vartheta_2 \frac{g}{n_1} \frac{2 n_1 n_2 \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1 n_2 \right) \xi_{12}
\]

\[
+ 2 \mu_1 \vartheta_2 \left( \frac{n_2^2 \Delta \mu}{\langle \mu \rangle} - \frac{g}{n_1} \frac{2 n_1 n_2 \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1 n_2 \right) \xi_{21}
\]

\[
+ 2 \mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{g}{n_1} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1 n_2 \right) \xi_{22}
\]

\[
(C^1 \xi)_{21} = (A^1 \xi)_{21} + \vartheta_2 (A^1 (\lambda \otimes n))_{21}
\]

\[
= 2 \mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1 n_2 \xi_{11}
\]

\[
+ 2 \mu_1 \vartheta_2 \frac{n_2^2 \Delta \mu}{\langle \mu \rangle} - \frac{g}{n_1} \frac{2 n_1 n_2 \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1 n_2 \xi_{12}
\]

\[
+ \left( 2 \mu_1 + 2 \mu_1 \vartheta_2 \frac{n_2^2 \Delta \mu}{\langle \mu \rangle} - 2 \mu_1 \vartheta_2 \frac{g}{n_1} \frac{2 n_1 n_2 \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1 n_2 \right) \xi_{21}
\]

\[
+ 2 \mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{g}{n_1} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1 n_2 \right) \xi_{22}
\]

\[
(C^1 \xi)_{22} = (A^1 \xi)_{22} + \vartheta_2 (A^1 (\lambda \otimes n))_{22}
\]

\[
= \left[ (\kappa_1 - \mu_1) + \vartheta_2 (\kappa_1 - \mu_1) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \mu \rangle} - \frac{g}{n_1} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_2^2 \right) \right] \xi_{11}
\]

\[
+ \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_2^2 \xi_{12}
\]

\[
+ \vartheta_2 2 n_1 n_2 \left[ - (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1^2 \right]
\]

\[
+ \vartheta_2 \left( \frac{\Delta \mu}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_2^2 \xi_{21}
\]

\[
+ \vartheta_2 2 n_1 n_2 \left[ - (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_1^2 \right] +
\]

\[
+ \vartheta_2 2 n_1 n_2 \left[ - (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \mu \rangle} - \frac{g}{n_1} \right) \frac{\Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_2^2 \right]
\]

\[
\]
From the last equations we obtain the $C_{ijkl}^{1}$:

\[
C_{1111} = (\mu_1 + \kappa_1) + \vartheta_2(\kappa_1 - \mu_1) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 + (6.132) \\
\vartheta_2(\mu_1 + \kappa_1) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_2^2 + (6.133)
\]

\[
C_{1112} = \vartheta_2 n_1 n_2 \left[ (\mu_1 + \kappa_1) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) \right] n_1^2 + (6.134)
\]

\[
C_{1121} = \vartheta_2 n_1 n_2 \left[ (\mu_1 + \kappa_1) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) \right] n_1^2 + (6.135)
\]

\[
C_{1122} = (\kappa_1 - \mu_1) + \vartheta_2(\mu_1 + \kappa_1) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 + (6.136)
\]

\[
C_{1211} = 2 \mu_1 \vartheta_2 \left( \frac{\langle \bar{\mu} \rangle}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.137)
\]

\[
C_{1212} = 2 \mu_1 + 2 \mu_1 \vartheta_2 \left( \frac{\langle \bar{\mu} \rangle}{\langle \bar{\mu} \rangle} \right) n_2^2 - 2 \mu_1 \vartheta_2 \left( \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.138)
\]

\[
C_{1221} = 2 \mu_1 \vartheta_2 \left( \frac{n_2^2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.139)
\]

\[
C_{1222} = 2 \mu_1 \vartheta_2 \left( \frac{\langle \bar{\mu} \rangle}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.140)
\]

\[
C_{2111} = 2 \mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.141)
\]

\[
C_{2112} = 2 \mu_1 \vartheta_2 \left( \frac{n_2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.142)
\]

\[
C_{2121} = 2 \mu_1 + 2 \mu_1 \vartheta_2 \left( \frac{n_2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.143)
\]

\[
C_{2122} = 2 \mu_1 \vartheta_2 \left( \frac{\langle \bar{\mu} \rangle}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.144)
\]

\[
C_{2211} = 2 \mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.145)
\]

\[
C_{2212} = 2 \mu_1 \vartheta_2 \left( \frac{n_2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.146)
\]

\[
C_{2221} = 2 \mu_1 \vartheta_2 \left( \frac{\langle \bar{\mu} \rangle}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) n_1^2 n_2 + (6.147)
\]

\[
C_{2222} = \vartheta_2 n_1 n_2 \left[ (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) \right] n_1^2 + (6.148)
\]

\[
C_{2222} = \vartheta_2 n_1 n_2 \left[ (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) \right] n_1^2 + (6.149)
\]

\[
C_{2222} = \vartheta_2 n_1 n_2 \left[ (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \right) \right] n_1^2 + (6.150)
\]
\[ C_{i=2221} = \vartheta_2 n_1 n_2 \left[ - (\kappa_1 - \mu_1) \frac{\Delta \mu}{\langle \bar{\mu} \rangle} \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} n_1^2 + (\mu_1 + \kappa_1) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{\Delta \mu}{n_2^2} \right) \right] \quad (6.151) \]

\[ C_{i=2222} = (\mu_1 + \kappa_1) + \vartheta_2 (\kappa_1 - \mu_1) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_1^2} \right) n_2^2 + \vartheta_2 (\mu_1 + \kappa_1) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_2^2} \right) \quad (6.152) \]

and analogously the \( C_{i=ijkl}^2 \)

\[ C_{i=1111} = (\mu_2 + \kappa_2) - \vartheta_1 (\mu_2 + \kappa_2) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_1^2} \right) n_1^2 \quad (6.154) \]

\[ \vartheta_1 (\kappa_2 - \mu_2) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_2^2} \right) n_2^2 \quad (6.155) \]

\[ C_{i=1112} = -\vartheta_1 n_1 n_2 \left[ (\mu_2 + \kappa_2) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{\Delta \mu}{n_1^2} \right) - (\kappa_2 - \mu_2) \left( \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{\Delta \mu}{n_2^2} \right) \right] \quad (6.156) \]

\[ C_{i=1121} = -\vartheta_1 n_1 n_2 \left[ - (\mu_2 + \kappa_2) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{\Delta \mu}{n_1^2} \right) n_2^2 + (\kappa_2 - \mu_2) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{\Delta \mu}{n_2^2} \right) \right] \quad (6.157) \]

\[ C_{i=1122} = (\kappa_2 - \mu_2) - \vartheta_1 (\mu_2 + \kappa_2) \left( \frac{\Delta \mu - \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_1^2} \right) n_1^2 \quad (6.158) \]

\[ \vartheta_1 (\kappa_2 - \mu_2) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_2^2} \right) n_2^2 \quad (6.159) \]

\[ C_{i=2111} = -2 \mu_2 \vartheta_1 \left( \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_1 n_2} \right) n_1 n_2 \quad (6.160) \]

\[ C_{i=2112} = 2 \mu_2 - 2 \mu_2 \vartheta_1 n_2^2 \frac{\Delta \mu}{\langle \bar{\mu} \rangle} + 2 \mu_2 \vartheta_1 \frac{\langle \bar{\kappa} \rangle}{n_1 n_2 \langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} n_1 n_2 \quad (6.161) \]

\[ C_{i=2121} = -2 \mu_2 \vartheta_1 \left( \frac{n_2^2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_1 n_2 \Delta \mu}{n_1 n_2} \right) n_1 n_2 \quad (6.162) \]

\[ C_{i=2122} = -2 \mu_2 \vartheta_1 \left( \frac{n_2^2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_1 n_2 \Delta \mu}{n_1 n_2} \right) n_1 n_2 \quad (6.163) \]

\[ C_{i=2111} = -2 \mu_2 \vartheta_1 \left( \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_1 n_2 \Delta \mu}{n_1 n_2} \right) n_1 n_2 \quad (6.164) \]

\[ C_{i=2112} = -2 \mu_2 \vartheta_1 \left( \frac{n_2^2 \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_1 n_2 \Delta \mu}{n_1 n_2} \right) n_1 n_2 \quad (6.165) \]

\[ C_{i=2121} = 2 \mu_2 - 2 \mu_2 \vartheta_1 n_2^2 \frac{\Delta \mu}{\langle \bar{\mu} \rangle} + 2 \mu_2 \vartheta_1 \frac{\langle \bar{\kappa} \rangle}{n_1 n_2 \langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} n_1 n_2 \quad (6.166) \]

\[ C_{i=2122} = -2 \mu_2 \vartheta_1 \left( \frac{\Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_1 n_2 \Delta \mu}{n_1 n_2} \right) n_1 n_2 \quad (6.167) \]

\[ C_{i=2211} = (\kappa_2 - \mu_2) - \vartheta_1 (\kappa_2 - \mu_2) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_1^2} \right) n_1^2 \quad (6.168) \]

\[ \vartheta_1 (\mu_2 + \kappa_2) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle} \frac{2 n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{n_2^2} \right) n_2^2 \quad (6.169) \]
The design variable are $\vartheta = \vartheta_1$ and $\gamma$. Then $\vartheta_2 = 1 - \vartheta$. Use that $n_1 = \cos \gamma$ and $n_2 = \sin \gamma$. We have

\[
\langle \bar{\mu} \rangle = \vartheta_2 \mu_1 + \vartheta_1 \mu_2 = (1 - \vartheta) \mu_1 + \vartheta \mu_2 = \mu_1 + (\mu_2 - \mu_1) \vartheta = \mu_1 + \Delta \mu \vartheta \tag{6.174}
\]

\[
\langle \bar{\kappa} \rangle = \kappa_1 + \Delta \kappa \vartheta \tag{6.175}
\]

\[
\langle \bar{\mu} \rangle + \langle \bar{\kappa} \rangle = \mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta. \tag{6.176}
\]

For the $C^{1}_{ijkl}$, we obtain

\[
C^{2}_{2212} = -\vartheta_1 2 n_1 n_2 \left[ (\kappa_2 - \mu_2) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{\Delta \mu}{\langle \bar{\mu} \rangle} n_1^2 \right) - (\mu_2 + \kappa_2) \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{\Delta \mu}{\langle \bar{\mu} \rangle} n_2^2 \right]. \tag{6.170}
\]

\[
C^{2}_{2221} = -\vartheta_1 2 n_1 n_2 \left[ -(\kappa_2 - \mu_2) \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{\Delta \mu}{\langle \bar{\mu} \rangle} n_1^2 + (\mu_2 + \kappa_2) \left( \frac{\Delta \mu}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{\Delta \mu}{\langle \bar{\mu} \rangle} n_2^2 \right) \right]. \tag{6.171}
\]

\[
C^{2}_{2222} = (\mu_2 + \kappa_2) - \vartheta_1 (\kappa_2 - \mu_2) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2 n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} + \Delta \kappa \right) n_1^2 \tag{6.172}
\]

\[
\vartheta_1 (\mu_2 + \kappa_2) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \bar{\mu} \rangle} - \frac{\langle \bar{\kappa} \rangle}{\langle \bar{\mu} \rangle} \frac{2 n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \bar{\mu} \rangle} n_1^2 \right) \tag{6.173}
\]
\begin{align}
C_{122}^1 & = \kappa_1 - \mu_1 + \vartheta_2(\mu_1 + \kappa_1) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_1^2 + \tag{6.191} \\
\vartheta_2(\kappa_1 - \mu_1) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_2^2 & = \kappa_1 - \mu_1 + (\mu_1 + \kappa_1)(\Delta \kappa - \Delta \mu) \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \cos^2 \gamma - \tag{6.192} \\
(\mu_1 + \kappa_1) \left( \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta)} \right) (-\Delta \mu \cos 2\gamma \cos^2 \gamma + \Delta \kappa \cos^2 \gamma) & + (6.194) \\
(\kappa_1 - \mu_1)(\Delta \kappa - \Delta \mu) \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin^2 \gamma & - \tag{6.195} \\
(\kappa_1 - \mu_1)(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta) \left( \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{\mu_1 + \Delta \mu \vartheta} \right) \left( \Delta \mu \sin 2\gamma \cos 2\gamma + \Delta \kappa \sin 2\gamma \right) & + (6.196) \\
C_{1211}^1 & = 2\mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_{11}^2 + \tag{6.197} \\
& = \mu_1 \Delta \kappa \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma & - \tag{6.198} \\
\mu_1 \left( \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta)} \right) \left( \Delta \mu \sin 2\gamma \cos 2\gamma + \Delta \kappa \sin 2\gamma \right) & + (6.199) \\
C_{1212}^1 & = 2\mu_1 + 2\mu_1 \vartheta_2 \frac{n_2^2 \Delta \mu}{\langle \mu \rangle} - 2\mu_1 \vartheta_2 \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_1 n_2 \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_{11}^2 + \tag{6.200} \\
& = 2\mu_1 + 2\mu_1 \Delta \mu \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin^2 \gamma - \tag{6.201} \\
\mu_1 \Delta \mu \left( \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta)} \right) \sin^2 2\gamma & + (6.202) \\
C_{1221}^1 & = 2\mu_1 \vartheta_2 \left( \frac{n_2^2 \Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_1 n_2 \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) + \tag{6.203} \\
& = 2\mu_1 \Delta \mu \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \cos^2 \gamma - \mu_1 \Delta \mu \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta)} \sin^2 2\gamma & + (6.204) \\
C_{1222}^1 & = 2\mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_{11}^2 + \tag{6.205} \\
& = \mu_1 \Delta \kappa \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma & - \tag{6.206} \\
\mu_1 \left( \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta)} \right) \left( \Delta \mu \sin 2\gamma \cos 2\gamma + \Delta \kappa \sin 2\gamma \right) & + (6.207) \\
C_{2111}^1 & = 2\mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_{11}^2 + \tag{6.208} \\
& = \mu_1 \Delta \kappa \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma & - \tag{6.209} \\
\mu_1 \left( \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta)} \right) \left( \Delta \mu \sin 2\gamma \cos 2\gamma + \Delta \kappa \sin 2\gamma \right) & + (6.210) \\
C_{2112}^1 & = 2\mu_1 \vartheta_2 \left( \frac{n_2^2 \Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{2n_1 n_2 \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) + \tag{6.211} \\
\end{align}
\[
C_{2121}^3 = 2\mu_1 + 2\mu_1\vartheta_2 n_2 \frac{n_2^2 \Delta \mu}{\langle \mu \rangle} - 2\mu_1\vartheta_2 \frac{\langle \kappa \rangle}{\langle \mu \rangle} 2n_1 n_2 \Delta \mu (\langle \mu \rangle + \langle \kappa \rangle) n_1 n_2
\]

\[
= 2\mu_1 + 2\mu_1 \Delta \mu \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta \cos^2 \gamma} - \mu_1 \Delta \mu \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin^2 2\gamma
\]

\[
C_{2122}^3 = 2\mu_1 \vartheta_2 \left( \frac{\Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} 2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu \right) n_1 n_2
\]

\[
= \mu_1 \Delta \kappa \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma
\]

\[
C_{2211}^3 = \kappa_1 - \mu_1 + \vartheta_2 (\kappa_1 - \mu_1) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} 2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu \right) n_1^2 + \vartheta_2 (\mu_1 + \kappa_1) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} 2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu \right) n_2^2
\]

\[
= \kappa_1 - \mu_1 + (\kappa_1 - \mu_1) (\Delta \mu + \Delta \kappa) \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \cos^2 \gamma - \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + \Delta \mu + \Delta \kappa \vartheta)} (-\Delta \mu \sin 2\gamma \cos 2\gamma + \Delta \kappa \sin 2\gamma)
\]

\[
C_{2212}^3 = \vartheta_2 n_1 n_2 \left[ (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{\Delta \mu}{\langle \mu \rangle} n_1^2 \right) - (\mu_1 + \kappa_1) \left( \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{\Delta \mu}{\langle \mu \rangle} n_2^2 \right) \right]
\]

\[
= (\kappa_1 - \mu_1) \Delta \mu \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma
\]

\[
C_{2221}^3 = \vartheta_2 n_1 n_2 \left[ - (\kappa_1 - \mu_1) \left( \frac{\Delta \mu}{\langle \mu \rangle} + \frac{\langle \kappa \rangle}{\langle \mu \rangle} n_1^2 \right) + (\mu_1 + \kappa_1) \left( \frac{\Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle}{\langle \mu \rangle} \frac{\Delta \mu}{\langle \mu \rangle} n_2^2 \right) \right]
\]

\[
= -(\kappa_1 - \mu_1) \Delta \mu \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma
\]
\[
\begin{align*}
C^{2}_{2222} & = (\mu_1 + \kappa_1) \vartheta_2(\kappa_1 - \mu_1) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \frac{2 n^2_2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n^1_1 + \\
& \quad \vartheta_2(\mu_1 + \kappa_1) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \frac{2 n^2_2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n^2_2 \\
& = \mu_1 + \kappa_1 + (\kappa_1 - \mu_1)(\Delta \kappa - \Delta \mu) \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \cos^2 \gamma - \\
& \quad \frac{(\kappa_1 - \mu_1)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa)\vartheta)} (-\Delta \mu \cos 2 \gamma \cos^2 \gamma + \Delta \kappa \cos^2 \gamma) \#(6.237) \\
& \quad (\mu_1 + \kappa_1)(\Delta \mu + \Delta \kappa) \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \sin^2 \gamma - \\
& \quad \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa)\vartheta)} (-\Delta \mu \cos 2 \gamma \sin^2 \gamma + \Delta \kappa \sin^2 \gamma) \#(6.239)
\end{align*}
\]

and for the $C^{2}_{ijkl}$

\[
\begin{align*}
C^{2}_{1111} & = (\mu_2 + \kappa_2) - \vartheta_1(\mu_2 + \kappa_2) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \frac{2 n^2_2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n^1_1 - \\
& \quad \vartheta_1(\kappa_2 - \mu_2) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \frac{2 n^2_2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n^2_2 \\
& = \mu_2 + \kappa_2 - (\mu_2 + \kappa_2)(\Delta \mu + \Delta \kappa) \frac{\vartheta}{\mu_1 + \Delta \mu \vartheta} \cos^2 \gamma + \\
& \quad \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa)\vartheta)} (\Delta \mu \cos 2 \gamma \cos^2 \gamma + \Delta \kappa \cos^2 \gamma) - (6.243) \\
& \quad (\mu_2 + \kappa_2)(\Delta \kappa - \Delta \mu) \frac{\vartheta}{\mu_1 + \Delta \mu \vartheta} \sin^2 \gamma + \\
& \quad \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa)\vartheta)} (\Delta \mu \cos 2 \gamma \sin^2 \gamma + \Delta \kappa \sin^2 \gamma) \\
& \quad (\kappa_2 - \mu_2)(\Delta \kappa - \Delta \mu) \frac{\vartheta}{\mu_1 + \Delta \mu \vartheta} \sin^2 \gamma + \\
& \quad \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa)\vartheta)} (\Delta \mu \cos 2 \gamma \sin^2 \gamma + \Delta \kappa \sin^2 \gamma)
\end{align*}
\]

\[
\begin{align*}
C^{2}_{1112} & = -\vartheta_1(\mu_2 + \kappa_2) \left( \frac{\Delta \mu}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} n^1_1 \right) - \vartheta_1(\kappa_2 - \mu_2) \left( \frac{\langle \tilde{\kappa} \rangle \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n^2_2 \\
& = -(\mu_2 + \kappa_2) \Delta \mu \frac{\vartheta}{\mu_1 + \Delta \mu \vartheta} \sin 2 \gamma + \\
& \quad (\mu_2 + \kappa_2) \Delta \mu \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{\mu_1 + \Delta \mu \vartheta} \cos^2 \gamma \sin 2 \gamma + \\
& \quad (\kappa_2 - \mu_2) \Delta \mu \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{\mu_1 + \Delta \mu \vartheta} \sin 2 \gamma \sin^2 \gamma \\
& \quad (\mu_2 + \kappa_2) \Delta \mu \frac{\vartheta}{\mu_1 + \Delta \mu \vartheta} \sin 2 \gamma \cos^2 \gamma \sin 2 \gamma - \\
& \quad (\kappa_2 - \mu_2) \Delta \mu \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{\mu_1 + \Delta \mu \vartheta} \sin 2 \gamma \sin^2 \gamma \\
& \quad (\kappa_2 - \mu_2) \Delta \mu \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{\mu_1 + \Delta \mu \vartheta} \sin 2 \gamma \sin^2 \gamma
\end{align*}
\]
\[ C_{122}^2 = \kappa_2 - \mu_2 - \vartheta_1(\mu_2 + \kappa_2) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle 2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_1^2 - (6.254) \]

\[ \vartheta_1(\kappa_2 - \mu_2) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle 2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_2^2 (6.255) \]

\[ = \kappa_2 - \mu_2 - (\mu_2 + \kappa_2)(\Delta \kappa - \Delta \mu) \frac{1}{\mu_1 + \Delta \mu \vartheta} \cos^2 \gamma + (6.256) \]

\[ \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_2 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa)\vartheta)} (\Delta \mu \cos 2\gamma \cos^2 \gamma + \Delta \kappa \cos^2 \gamma) - (6.257) \]

\[ (\kappa_2 - \mu_2)(\Delta \mu + \Delta \kappa) \frac{1}{\mu_1 + \Delta \mu \vartheta} \sin^2 \gamma + (6.258) \]

\[ \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{\mu_1 + \Delta \mu \vartheta} (\Delta \mu \sin 2\gamma \cos \gamma + \Delta \kappa \sin \gamma) + (6.259) \]

\[ C_{1211}^2 = -2\mu_2 \vartheta_1 \left( \frac{\Delta \kappa}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle 2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_1 n_2 (6.260) \]

\[ = -\mu_2 \Delta \kappa \frac{1}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma + (6.261) \]

\[ \mu_2 \frac{1}{\mu_1 + \Delta \mu \vartheta} (\Delta \mu \sin 2\gamma \cos \gamma + \Delta \kappa \sin \gamma) (6.262) \]

\[ C_{1212}^2 = 2\mu_2 - 2\mu_2 \vartheta_1 \frac{n_2^3 \Delta \mu}{\langle \tilde{\mu} \rangle} + 2\mu_2 \vartheta_1 \langle \tilde{\kappa} \rangle 2n_2^2 \Delta \mu \frac{n_1 n_2 \Delta \mu}{\langle \tilde{\mu} \rangle} n_1 n_2 (6.263) \]

\[ = 2\mu_2 - 2\mu_2 \Delta \mu \frac{1}{\mu_1 + \Delta \mu \vartheta} \sin^2 \gamma + (6.264) \]

\[ \mu_2 \Delta \mu \frac{1}{\mu_1 + \Delta \mu \vartheta} \frac{1}{\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa)\vartheta} \sin^2 2\gamma (6.265) \]

\[ C_{1221}^2 = -2\mu_2 \vartheta_1 \left( \frac{n_2^3 \Delta \mu}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle 2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_1 n_2 (6.266) \]

\[ = -\mu_2 \Delta \kappa \frac{1}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma + (6.266) \]

\[ \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{\mu_1 + \Delta \mu \vartheta} (\Delta \mu \sin 2\gamma \cos \gamma + \Delta \kappa \sin \gamma) (6.270) \]

\[ C_{1222}^2 = -2\mu_2 \vartheta_1 \left( \frac{\Delta \kappa}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle 2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_1 n_2 (6.268) \]

\[ \mu_2 \frac{1}{\mu_1 + \Delta \mu \vartheta} (\Delta \mu \sin 2\gamma \cos \gamma + \Delta \kappa \sin \gamma) (6.271) \]

\[ C_{2111}^2 = -2\mu_2 \vartheta_1 \left( \frac{\Delta \kappa}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle 2n_2^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_1 n_2 (6.271) \]

\[ = -\mu_2 \Delta \kappa \frac{1}{\mu_1 + \Delta \mu \vartheta} \sin 2\gamma + (6.272) \]

\[ \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{\mu_1 + \Delta \mu \vartheta} (\Delta \mu \sin 2\gamma \cos \gamma + \Delta \kappa \sin \gamma) (6.273) \]

\[ C_{2112}^2 = -2\mu_2 \vartheta_1 \left( \frac{n_2^3 \Delta \mu}{\langle \tilde{\mu} \rangle} - \frac{\langle \tilde{\kappa} \rangle 2n_2^2 \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_1 n_2 (6.274) \]
\[
\begin{align*}
C_{2121}^2 &= 2\mu_2 - 2\mu_2\vartheta_1 \frac{n_2^2\mu_1 + \Delta_22}{\mu_2 + \Delta_22} n_2 - 2\mu_2\vartheta_1 (\mu_2 - \mu_2)(\Delta_122 + \Delta_122) n_2^2 - 2\mu_2\vartheta_1 \frac{n_2^2\mu_1 + \Delta_22}{\mu_2 + \Delta_22} n_2 - 2\mu_2\vartheta_1 (\mu_2 - \mu_2)(\Delta_122 + \Delta_122) n_2^2.
\end{align*}
\]
We have that for $m$.

The effective tensor is given by

$$C_{2222}^2 = \mu_2 + \kappa_2 - \vartheta_1(\kappa_2 - \mu_2) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \hat{\mu} \rangle} - \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right) n_1^2 - \vartheta_1(\mu_2 + \kappa_2) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \hat{\mu} \rangle} - \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right) n_2^2.$$

We have that for $m = 1, 2$

$$C_{1211}^m = C_{2111}^m,$$  
$$C_{1222}^m = C_{2221}^m,$$  
$$C_{1212}^m = 2 \mu_m + C_{2112}^m,$$  
$$C_{2121}^m = 2 \mu_m + C_{2121}^m.$$  

The effective tensor is given by $C^E = \vartheta_1 C^1 + \vartheta_2 C^2 = \vartheta C^1 + (1 - \vartheta) C^2$. For the $C_{i,j,k,l}^E$ we obtain

$$C_{1111}^E = \vartheta_1(\mu_1 + \kappa_1) + \vartheta_2(\mu_2 + \kappa_2) - \bar{\vartheta}_1 \bar{\vartheta}_2 (\Delta \mu + \Delta \kappa) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \hat{\mu} \rangle} - \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right) n_1^2 - \bar{\vartheta}_1 \bar{\vartheta}_2 (\Delta \mu + \Delta \kappa) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \hat{\mu} \rangle} - \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right) n_2^2.$$

$$C_{1122}^E = \vartheta_1 \vartheta_2 n_1 n_2 \frac{\Delta \mu}{\langle \hat{\mu} \rangle} \left[ -(\Delta \mu + \Delta \kappa) \left( 1 - \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right) + (\Delta \kappa - \Delta \mu) \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right] + (\Delta \kappa - \Delta \mu) \langle \hat{\kappa} \rangle n_2^2 - (\Delta \kappa - \Delta \mu) \left( 1 - \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right) n_1^2.$$

$$C_{1212}^E = \vartheta_1 \vartheta_2 n_1 n_2 \frac{\Delta \mu}{\langle \hat{\mu} \rangle} \left[ \left( \frac{\Delta \mu + \Delta \kappa}{\langle \hat{\mu} \rangle} \right) - \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right] n_1^2 - \vartheta_1 \vartheta_2 (\Delta \mu + \Delta \kappa) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \hat{\mu} \rangle} - \frac{\langle \hat{\mu} \rangle}{\langle \hat{\mu} \rangle} \right) n_2^2.$$
Next we show that the effective elastic tensor is symmetric. Compute the following using the fact that
\[ C_{1211}^{E} = \vartheta_{1} \vartheta_{2} 2n_{1} n_{2} \frac{\Delta \mu}{\langle \mu \rangle} \left[ \Delta \kappa + \langle \kappa \rangle \frac{2n_{2}^{2}\Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right] \] (6.311)
\[ C_{1212}^{E} = 2\mu_{1} \vartheta_{1} + 2\mu_{2} \vartheta_{2} - 2\Delta \mu \vartheta_{1} \vartheta_{2} \frac{n_{2}^{2}\Delta \mu}{\langle \mu \rangle} + 2\Delta \mu \vartheta_{1} \vartheta_{2} \frac{\langle \kappa \rangle 2n_{1} n_{2} \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_{1} n_{2} \] (6.312)
\[ C_{1221}^{E} = -2\Delta \mu \vartheta_{1} \vartheta_{2} \left( \frac{n_{2}^{2}\Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle 2n_{1} n_{2} \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} n_{1} n_{2} \right) \] (6.313)
\[ C_{1222}^{E} = \vartheta_{1} \vartheta_{2} 2n_{1} n_{2} \frac{\Delta \mu}{\langle \mu \rangle} \left[ -\Delta \kappa + \langle \kappa \rangle \frac{2n_{2}^{2}\Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right] \] (6.314)
\[ C_{2211}^{E} = \vartheta_{1}(\kappa_{1} - \mu_{1}) + \vartheta_{2}(\kappa_{2} - \mu_{2}) - \] (6.315)
\[ \vartheta_{1} \vartheta_{2} (\Delta \kappa - \Delta \mu) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle 2n_{2}^{2}\Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_{1}^{2} - \]
\[ \vartheta_{1} \vartheta_{2} (\Delta \mu + \Delta \kappa) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle 2n_{2}^{2}\Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_{2}^{2} \]
\[ C_{2212}^{E} = \vartheta_{1} \vartheta_{2} 2n_{1} n_{2} \frac{\Delta \mu}{\langle \mu \rangle} \left[ -\left( \Delta \kappa - \Delta \mu \right) \left( 1 - \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} n_{1}^{2} \right) + (\Delta \mu + \Delta \kappa) \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} n_{2}^{2} \right] \] (6.316)
\[ C_{2221}^{E} = \vartheta_{1} \vartheta_{2} 2n_{1} n_{2} \frac{\Delta \mu}{\langle \mu \rangle} \left[ (\Delta \kappa - \Delta \mu) \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} n_{1}^{2} - (\Delta \mu + \Delta \kappa) \left( 1 - \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} n_{2}^{2} \right) \right] \] (6.317)
\[ C_{2222}^{E} = \vartheta_{1}(\mu_{1} + \kappa_{1}) + \vartheta_{2}(\mu_{2} + \kappa_{2}) - \] (6.318)
\[ \vartheta_{1} \vartheta_{2} (\Delta \kappa - \Delta \mu) \left( \frac{\Delta \mu + \Delta \kappa}{\langle \mu \rangle} - \frac{\langle \kappa \rangle 2n_{2}^{2}\Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_{1}^{2} - \]
\[ \vartheta_{1} \vartheta_{2} (\Delta \mu + \Delta \kappa) \left( \frac{\Delta \kappa - \Delta \mu}{\langle \mu \rangle} - \frac{\langle \kappa \rangle 2n_{2}^{2}\Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_{2}^{2}. \]

Next we show that the effective elastic tensor is symmetric. Compute the following using the fact that \( n_{1}^{2} + n_{2}^{2} = 1 \) and \( 2n_{2}^{2} - 1 = -(2n_{1}^{2} - 1) \)

\[ \frac{1}{2}(C_{1112}^{E} + C_{1121}^{E}) = \vartheta_{1} \vartheta_{2} 2n_{1} n_{2} \frac{\Delta \mu}{\langle \mu \rangle} \left[ -\Delta \kappa + (\Delta \mu + \Delta \kappa) \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} n_{1}^{2} + \right. \] (6.319)
\[ \left. (\Delta \kappa - \Delta \mu) \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} (1 - n_{1}^{2}) \right] \] (6.320)
\[ \frac{1}{2}(C_{2212}^{E} + C_{2221}^{E}) = \vartheta_{1} \vartheta_{2} 2n_{1} n_{2} \frac{\Delta \mu}{\langle \mu \rangle} \left[ -\Delta \kappa + (\Delta \mu - \Delta \kappa) \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} + \right. \] (6.321)
\[ \left. (\Delta \mu + \Delta \kappa) \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} n_{2}^{2} \right] \] (6.322)
\[ \frac{1}{2}(C_{2222}^{E} + C_{2211}^{E}) = \vartheta_{1} \vartheta_{2} 2n_{1} n_{2} \frac{\Delta \mu}{\langle \mu \rangle} \left[ -\Delta \kappa + (\Delta \mu - \Delta \kappa) \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} (1 - n_{2}^{2}) + \right. \] (6.323)
\[ \left. (\Delta \mu + \Delta \kappa) \frac{\langle \kappa \rangle}{\langle \mu \rangle + \langle \kappa \rangle} n_{1}^{2} \right] \] (6.324)
\[ C_{1122}^{E} - C_{2211}^{E} = \vartheta_{1} \vartheta_{2} (\Delta \mu + \Delta \kappa) \left( \frac{\langle \kappa \rangle 2n_{2}^{2}\Delta \mu + \Delta \kappa - \Delta \mu}{\langle \mu \rangle + \langle \kappa \rangle} \right) n_{1}^{2} + \] (6.325)
\[ \vartheta_1 \vartheta_2 (\Delta \kappa - \Delta \mu) \left( \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \frac{2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_2^2 - \] (6.326)

\[ \vartheta_1 \vartheta_2 (\Delta \kappa - \Delta \mu) \left( \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \frac{2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_1^2 - \] (6.327)

\[ \vartheta_1 \vartheta_2 (\Delta \mu + \Delta \kappa) \left( \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \frac{2n_1^2 \Delta \mu + \Delta \kappa - \Delta \mu}{\langle \tilde{\mu} \rangle + \langle \tilde{\kappa} \rangle} \right) n_2^2 \] (6.328)

\[
\begin{align*}
\vartheta_1 \vartheta_2 \left( \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} + \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \right) & \left[ \left( \Delta \mu + \Delta \kappa \right) \left( -(2n_1^2 - 1) \Delta \mu + \Delta \kappa \right) \right] - \\
& \left( \Delta \kappa - \Delta \mu \right) \left( (2n_1^2 - 1) \Delta \mu + \Delta \kappa \right) n_1^2 + \\
\vartheta_1 \vartheta_2 \left( \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} + \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \right) & \left[ \left( \Delta \kappa - \Delta \mu \right) \left( -(2n_1^2 - 1) \Delta \mu + \Delta \kappa \right) \right] \left( 1 - n_1^2 \right) - \\
& \vartheta_1 \vartheta_2 \left( \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} + \frac{\langle \tilde{\kappa} \rangle}{\langle \tilde{\mu} \rangle} \right) \left[ 4(1 - n_1^2) \Delta \mu \Delta \kappa n_1^2 - 4n_1^2 \Delta \mu \Delta \kappa (1 - n_1^2) \right] = 0. \quad (6.333)
\end{align*}
\]

From equations (6.305) and (6.306) we obtain

\[
\frac{1}{2} (C^E_{1212} + C^E_{1221}) = \frac{1}{2} (2\mu_1 \vartheta_1 + 2\mu_2 \vartheta_2 + C^E_{2112} - 2\mu_1 \vartheta_1 - 2\mu_2 \vartheta_2 + C^E_{2121}) = \frac{1}{2} (C^E_{2112} + C^E_{2121}). \quad (6.334)
\]

Summarizing the above we find

\[
\begin{align*}
\frac{1}{2} (C^E_{1112} + C^E_{1121}) &= C^E_{1211} = C^E_{2111} \\
\frac{1}{2} (C^E_{2212} + C^E_{2221}) &= C^E_{1222} = C^E_{2122} \\
C^E_{1122} &= C^E_{2211} \\
\frac{1}{2} (C^E_{2112} + C^E_{2121}) &= \frac{1}{2} (C^E_{2112} + C^E_{2121}).
\end{align*}
\] (6.335, 6.336, 6.337, 6.338)

What is left to do is to find formulas for the elements of the macrostress modulation tensor \(Q\). To achieve this we start by computing \(|C^i \xi|^2\)

\[
C^i \xi : C^i \xi = \left( C^i_{1111} \xi_{11} + C^i_{1112} \xi_{12} + C^i_{1121} \xi_{21} + C^i_{1222} \xi_{22} \right)^2 + \\
\left( C^i_{2211} \xi_{11} + C^i_{2212} \xi_{12} + C^i_{2121} \xi_{21} + C^i_{2222} \xi_{22} \right)^2 + \\
\left( C^i_{2111} \xi_{11} + C^i_{2112} \xi_{12} + C^i_{2122} \xi_{22} \right)^2 + \\
\left( C^i_{2211} \xi_{11} + C^i_{2212} \xi_{12} + C^i_{2221} \xi_{21} + C^i_{2222} \xi_{22} \right)^2. \quad (6.339)
\]

From equation (6.339) we finally obtain for the \(Q^i_{ijkl}\)

\[
\begin{align*}
Q^i_{1111} &= C^i_{1111} + C^i_{1211} + C^i_{2111} + C^i_{2211} \\
Q^i_{1112} = Q^i_{1211} &= C^i_{1111} C^i_{1112} + C^i_{1121} C^i_{1212} + C^i_{2111} C^i_{2112} + C^i_{2211} C^i_{2212} \\
Q^i_{1121} = Q^i_{2111} &= C^i_{1111} C^i_{1121} + C^i_{1211} C^i_{1221} + C^i_{2111} C^i_{2121} + C^i_{2211} C^i_{2221} \\
Q^i_{1122} = Q^i_{2211} &= C^i_{1111} C^i_{1122} + C^i_{1211} C^i_{1222} + C^i_{2111} C^i_{2122} + C^i_{2211} C^i_{2222} \\
Q^i_{1212} &= C^i_{1111} + C^i_{1211} + C^i_{2112} + C^i_{2212} \\
\end{align*} \] (6.340, 6.341, 6.342, 6.343, 6.344)
\begin{align*}
Q_{1221}^i &= Q_{1212}^i = C_{1112}^i C_{1121}^i + C_{1212}^i C_{1221}^i + C_{2112}^i C_{2121}^i + C_{2212}^i C_{2221}^i 
&= (6.345) \\
Q_{1222}^i &= Q_{2212}^i = C_{1112}^i C_{1212}^i + C_{1212}^i C_{1222}^i + C_{2112}^i C_{2212}^i + C_{2212}^i C_{2222}^i 
&= (6.346) \\
Q_{2121}^i &= C_{1121}^i + C_{2121}^i + C_{2121}^i + C_{2212}^i 
&= (6.347) \\
Q_{2122}^i &= Q_{2211}^i = C_{1121}^i C_{1212}^i + C_{1221}^i C_{1222}^i + C_{2121}^i C_{2212}^i + C_{2211}^i C_{2222}^i 
&= (6.348) \\
Q_{2222}^i &= C_{1222}^i + C_{2122}^i + C_{2122}^i + C_{2222}^i 
&= (6.349)
\end{align*}

6.2 Sensitivity Analysis

To find the updates given in section 5.3 we have to compute the derivatives of the stiffness tensor and the macrostress modulation tensor with respect to the design variables. In this section formulas for the derivatives are given.

\[
\frac{\partial}{\partial \vartheta} \left( \frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \right) = \frac{-\mu_1 - \Delta \mu \vartheta - (1 - \vartheta) \Delta \mu}{(\mu_1 + \Delta \mu \vartheta)^2} = -\frac{\mu_1 + \Delta \mu}{(\mu_1 + \Delta \mu \vartheta)^2} = -\frac{\mu_2}{(\mu_1 + \Delta \mu \vartheta)^2} 
\]

\[
\frac{\partial}{\partial \vartheta} \left( \frac{\vartheta}{\mu_1 + \Delta \mu \vartheta} \right) = \frac{\mu_1 + \Delta \mu \vartheta - \vartheta \Delta \mu}{(\mu_1 + \Delta \mu \vartheta)^2} = \frac{\mu_1}{(\mu_1 + \Delta \mu \vartheta)^2} 
\]

\[
f_1(\vartheta) = \frac{(1 - \vartheta)(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta)} = \frac{\kappa_1 - \kappa_2 \vartheta - \Delta \kappa \vartheta^2}{\mu_1(\mu_1 + \kappa_1) + [\Delta \mu(\mu_1 + \kappa_1) + \mu_1(\Delta \mu + \Delta \kappa)] \vartheta + \Delta \mu(\Delta \mu + \Delta \kappa) \vartheta^2} = \frac{u_1(\vartheta)}{v(\vartheta)} \] 

\[
f_2(\vartheta) = \frac{\vartheta(\kappa_1 + \Delta \kappa \vartheta)}{(\mu_1 + \Delta \mu \vartheta)(\mu_1 + \kappa_1 + (\Delta \mu + \Delta \kappa) \vartheta)} \] 

\[
\frac{\partial u_1}{\partial \vartheta} = -\kappa_2 - 2\Delta \kappa \vartheta 
\]

\[
\frac{\partial u_2}{\partial \vartheta} = \kappa_1 - 2\Delta \kappa \vartheta 
\]

\[
\frac{\partial v}{\partial \vartheta} = \Delta \mu(\mu_1 + \kappa_1) + \mu_1(\Delta \mu + \Delta \kappa) + 2\Delta \mu(\Delta \mu + \Delta \kappa) \vartheta 
\]

\[
\frac{\partial f_1}{\partial \vartheta} = \frac{u_1' v - u_1 v'}{v^2} 
\]

\[
\frac{\partial f_2}{\partial \vartheta} = \frac{u_2' v - u_2 v'}{v^2} 
\]

Because of the special structure of the formulas for the stiffness tensor it is enough to replace in equations (6.177)-(6.302)

\[
\frac{1 - \vartheta}{\mu_1 + \Delta \mu \vartheta} \quad \text{by} \quad -\frac{\mu_2}{(\mu_1 + \Delta \mu \vartheta)^2} 
\]

\[
\frac{\vartheta}{\mu_1 + \Delta \mu \vartheta} \quad \text{by} \quad \frac{\mu_1}{(\mu_1 + \Delta \mu \vartheta)^2} 
\]

\[
f_1(\vartheta) \quad \text{by} \quad \frac{\partial f_1}{\partial \vartheta} 
\]

\[
f_2(\vartheta) \quad \text{by} \quad \frac{\partial f_2}{\partial \vartheta} 
\]

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to obtain the derivatives \( \frac{\partial C_{ijkl}^m}{\partial \gamma} \). To obtain \( \frac{\partial C_{ijkl}^m}{\partial \gamma} \) replace the trigonometric expressions with their derivatives given in (6.361)-(6.370)

\[
\frac{\partial}{\partial \gamma} \sin^2 \gamma = 2 \sin \gamma \cos \gamma = \sin 2\gamma \quad (6.361)
\]

\[
\frac{\partial}{\partial \gamma} \cos^2 \gamma = -2 \sin \gamma \cos \gamma = -\sin 2\gamma \quad (6.362)
\]

\[
\frac{\partial}{\partial \gamma} \sin 2\gamma = 2 \cos 2\gamma \quad (6.363)
\]

\[
\frac{\partial}{\partial \gamma} \cos 2\gamma = -2 \sin 2\gamma \quad (6.364)
\]

\[
\frac{\partial}{\partial \gamma} \sin^2 2\gamma = 4 \sin 2\gamma \cos 2\gamma = 2 \sin 4\gamma \quad (6.365)
\]

\[
\frac{\partial}{\partial \gamma} \sin 2\gamma \sin^2 \gamma = 2 \cos 2\gamma \sin^2 \gamma + \sin^2 2\gamma \quad (6.366)
\]

\[
\frac{\partial}{\partial \gamma} \sin 2\gamma \cos^2 \gamma = 2 \cos 2\gamma \cos^2 \gamma - \sin^2 2\gamma \quad (6.367)
\]

\[
\frac{\partial}{\partial \gamma} \cos 2\gamma \sin^2 \gamma = -2 \sin 2\gamma \sin^2 \gamma + \cos 2\gamma \sin 2\gamma = \sin 4\gamma - \sin 2\gamma \quad (6.368)
\]

\[
\frac{\partial}{\partial \gamma} \cos 2\gamma \cos^2 \gamma = -2 \sin 2\gamma \cos^2 \gamma - \cos 2\gamma \sin 2\gamma = -\sin 4\gamma - \sin 2\gamma \quad (6.369)
\]

\[
\frac{\partial}{\partial \gamma} \sin 2\gamma \cos 2\gamma = 2(\cos^2 2\gamma - \sin^2 2\gamma) = 2 \cos 4\gamma. 
\quad (6.370)
\]

This establishes the derivatives of the stiffness tensor. For the macrostress modulation tensor we obtain for \( \frac{\partial Q_{ijkl}}{\partial C_{ij}} \), \( \zeta_1 = \theta \), \( \zeta_2 = \gamma \)

\[
\partial_\theta Q_{1111}^i = 2(C_{1111}^i \partial_\theta \gamma \partial_\theta \zeta_2 C_{1111}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1111}^i + C_{2111}^i \partial_\theta \zeta_1 C_{2111}^i + C_{2211}^i \partial_\theta \zeta_1 C_{2211}^i ) \quad (6.371)
\]

\[
\partial_\theta Q_{1112}^i = \partial_\theta Q_{1211}^i = \partial_\theta C_{1111}^i C_{1112}^i + C_{1111}^i \partial_\theta \zeta_1 C_{1112}^i + \partial_\theta C_{1111}^i \partial_\theta \zeta_1 C_{1112}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i \quad (6.372)
\]

\[
\partial_\theta Q_{1121}^i = \partial_\theta Q_{1211}^i = \partial_\theta C_{1111}^i C_{1211}^i + C_{1111}^i \partial_\theta \zeta_1 C_{1211}^i + \partial_\theta C_{1111}^i \partial_\theta \zeta_1 C_{1211}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i \quad (6.373)
\]

\[
\partial_\theta Q_{1122}^i = \partial_\theta Q_{2211}^i = \partial_\theta C_{1111}^i C_{1212}^i + C_{1111}^i \partial_\theta \zeta_1 C_{1212}^i + \partial_\theta C_{1111}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i \quad (6.374)
\]

\[
\partial_\theta Q_{1212}^i = \partial_\theta Q_{2212}^i = \partial_\theta C_{1112}^i C_{1212}^i + C_{1112}^i \partial_\theta \zeta_1 C_{1212}^i + \partial_\theta C_{1112}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i \quad (6.375)
\]

\[
\partial_\theta Q_{1221}^i = \partial_\theta Q_{2211}^i = \partial_\theta C_{1112}^i C_{1212}^i + C_{1112}^i \partial_\theta \zeta_1 C_{1212}^i + \partial_\theta C_{1112}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i \quad (6.376)
\]

\[
\partial_\theta Q_{1222}^i = \partial_\theta Q_{2212}^i = \partial_\theta C_{1112}^i C_{1212}^i + C_{1112}^i \partial_\theta \zeta_1 C_{1212}^i + \partial_\theta C_{1112}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i \quad (6.377)
\]

\[
\partial_\theta Q_{2121}^i = 2(C_{1121}^i \partial_\theta \zeta_1 C_{1111}^i + C_{1121}^i \partial_\theta \zeta_1 C_{1112}^i + C_{2121}^i \partial_\theta \zeta_1 C_{2111}^i + C_{2121}^i \partial_\theta \zeta_1 C_{2112}^i + C_{2121}^i \partial_\theta \zeta_1 C_{2211}^i + C_{2121}^i \partial_\theta \zeta_1 C_{2212}^i) \quad (6.378)
\]

\[
\partial_\theta Q_{2122}^i = \partial_\theta Q_{2221}^i = \partial_\theta C_{1121}^i C_{1212}^i + C_{1121}^i \partial_\theta \zeta_1 C_{1212}^i + \partial_\theta C_{1121}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i + C_{1211}^i \partial_\theta \zeta_1 C_{1212}^i \quad (6.379)
\]

\[
\partial_\theta Q_{2222}^i = 2(C_{1122}^i \partial_\theta \zeta_1 C_{1112}^i + C_{1122}^i \partial_\theta \zeta_1 C_{1112}^i + C_{2122}^i \partial_\theta \zeta_1 C_{2122}^i + C_{2122}^i \partial_\theta \zeta_1 C_{2222}^i) \quad (6.380)
\]
7. Numerical Methods

7.1 The Finite Element Method
This chapter presents the numerical tools to solve the problems described in chapters 3 through 5. A common way to solve elliptic boundary value problems is the Finite Element Method. We show the method for the torsional rigidity and the plane strain problem and describe how to solve the resulting systems of linear equations by iterative methods.

7.1.1 The Scalar Case of Torsional Rigidity
In this section we show the discretization of the torsional rigidity problem. Given a two dimensional domain \( \Omega \) with boundary \( \Gamma \). Note that in the following all functions depend on the two spatial variables \( x_1 \) and \( x_2 \) even if not written explicitly, i.e. \( u = u(x_1, x_2) \). Compute the solution \( u \) of the problem

\[
\begin{align*}
- \text{div} \, S \nabla u &= f \quad \text{in } \Omega \\
 u &= g_D \quad \text{at } \Gamma_D \\
 n \cdot (S \nabla u) &= g_N \quad \text{at } \Gamma_N
\end{align*}
\]  

(7.1)

where \( \Gamma_D \cup \Gamma_N = \Gamma \), \( \Gamma_D \cap \Gamma_N = \emptyset \), and \( n \) is the outward unit normal vector at the boundary. Multiplying the PDE in (7.1) with a test function \( w \) and integrating over the domain \( \Omega \) gives

\[
- \int_\Omega \text{div} \, S \nabla u \, w \, dx = \int_\Omega f \, w \, dx.
\]

(7.2)

Using integration by parts on the left hand side we obtain

\[
\int_\Omega S \nabla u \nabla w \, dx - \int_\Gamma n \cdot (S \nabla u) \, w \, ds = \int_\Omega f \, w \, dx.
\]

(7.3)

Replacing the boundary integral with the Neumann boundary condition from (7.1) leads to

\[
\int_\Omega S \nabla u \nabla w \, dx - \int_\Gamma g_N \, w \, ds = \int_\Omega f \, w \, dx.
\]

(7.4)

A finite decomposition of the domain \( \Omega \) is given by

\[
\Omega = \bigcup_{K \in \mathcal{T}_h} K
\]

(7.5)

where

- \( K \) is a polyhedron
- \( K_1 \cup K_2 = \emptyset \) for each distinct polyhedrons \( K_1, K_2 \)
- \( h \) is a parameter representing the level of refinement, \( \text{diam}(K) \leq h \) for each \( K \in \mathcal{T}_h \).

In what follows we do not want to consider general polyhedrons but only triangles and squares. We expect the solution \( u \) of problem (7.1) to be in a subspace \( X \) of the Sobolev space \( H^1(\Omega) \). As a finite dimensional space which suitably approximates the infinite dimensional space \( X \) we choose the space
of piecewise polynomials. The basis functions for the space $X_h$ are called shape functions (see section 7.1.5). In the space $X_h$ equation (7.4) becomes

$$\sum_i \int_{\Omega_i} S_i \nabla u_h \nabla w_h \, dx = \sum_i \int_{\Omega_i} f_i w_h \, dx + \sum_j \int_{\Gamma_j} g_j w_h \, ds$$

(7.6)

We express $u_h$ and $w_h$ over each element domain $\Omega_e$ by those shape functions $H_i$, $i = 1 \ldots n$. Here we have that and $n = \frac{(m+1)(m+2)}{2}$ for triangles, $n = \frac{(m+1)(m+2)+2m}{2}$ for rectangles, and $m$ is the degree of the shape functions over each finite element.

$$u_h = \sum_{i=1}^n u_i H_i$$

(7.7)

$$w_h = \sum_{j=1}^n H_j.$$  

(7.8)

So we obtain for $S_h \nabla u_h$ and $\nabla w_h$

$$S_h \nabla u_h = \sum_{i=1}^n S_i u_i \nabla H_i$$

(7.9)

$$\nabla w_h = \sum_{j=1}^n \nabla H_j.$$  

(7.10)

For an element domain $\Omega_e$ we have for the first term of (7.6)

$$\int_{\Omega_e} S_h \nabla u_h \nabla w_h \, dx = \int_{\Omega_e} \sum_{i=1}^n S_i u_i \nabla H_i \sum_{j=1}^n \nabla H_j \, dx$$

(7.11)

$$= \int_{\Omega_e} (u_1 \ldots u_n) \cdot \begin{pmatrix} S_1 \nabla H_1 \\ \vdots \\ S_n \nabla H_n \end{pmatrix} \odot (\nabla H_1 \ldots \nabla H_n) \, dx$$

(7.12)

$$= \int_{\Omega_e} \begin{pmatrix} S_1 \nabla H_1 \nabla H_1 & \ldots & S_n \nabla H_1 \nabla H_n \\ \vdots & \ddots & \vdots \\ S_n \nabla H_n \nabla H_1 & \ldots & S_n \nabla H_n \nabla H_n \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} \, dx$$

(7.13)

$$= \begin{pmatrix} \int_{\Omega_e} S_1 \nabla H_1 \nabla H_1 \, dx & \ldots & \int_{\Omega_e} S_n \nabla H_1 \nabla H_n \, dx \\ \vdots & \ddots & \vdots \\ \int_{\Omega_e} S_1 \nabla H_n \nabla H_1 \, dx & \ldots & \int_{\Omega_e} S_n \nabla H_n \nabla H_n \, dx \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}.$$  

(7.14)

The forcing term at an element domain can be written as

$$\int_{\Omega_e} f_h w_h \, dx = \int_{\Omega_e} (f_1 H_1 \ldots f_n H_n)^T \, dx = (f_1 \int_{\Omega_e} H_1 \, dx \ldots f_n \int_{\Omega_e} H_n \, dx)^T.$$  

(7.15)

The boundary term of (7.6) at a boundary element can be computed as follows

$$\int_{\Gamma_j} g_h w_h \, ds = \int_{\Gamma_j} (g_1 H_1 \ldots g_m H_m)^T \, ds = (g_1 \int_{\Gamma_j} H_1 \, ds \ldots g_m \int_{\Gamma_j} H_m \, ds)^T$$

(7.16)
where $m$ represents the number of boundary points of the finite element of degree of freedom $n$. We call the element matrix in (7.14) $A^e_i$ and the sum of the two vectors (7.15) and (7.16) $b^e_i$. Then on the element $\Omega^e_i$ holds

$$A^e_i u_i = b^e_i. \tag{7.17}$$

Assembling over all elements $\Omega^e_i$ we can write (7.6) as

$$Au = b. \tag{7.18}$$

There are two ways to handle the remaining Dirichlet boundary conditions. Because on the Dirichlet boundary the solution $u|_{\Gamma_D}$ is given explicitly the first way is to eliminate those points from the system (7.18).

The second way is a penalty method. The Dirichlet conditions $u|_{\Gamma_D} = g^D$ are approximated by adding a term

$$Lu|_{\Gamma_D} = Lg^D \tag{7.19}$$

to the system (7.18) where is a large number such as $10^4$ times the largest entry of $A$. By increasing $L$ the Dirichlet conditions are approximated more accurately but on the other hand a potential ill-conditioning of the system increases the number of iterations to solve it.

### 7.1.2 Reformulation of the Plane Strain Problem

In the plane strain problem (5.1) in chapter 5 the stiffness tensor and the stress amplification tensor are fourth order tensors and the stresses and strains matrices. To simplify the problem one can rewrite the $2 \times 2$ stress and strain matrix as a 3D vector because of symmetry. We have writing the displacement $u = (u, v)^T$

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{pmatrix} \rightarrow \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \end{pmatrix} \begin{pmatrix} \frac{\partial x_1 u}{2} & \frac{\partial x_2 v}{2} \\ \frac{\partial x_2 u}{2} & \frac{\partial x_1 v}{2} \end{pmatrix} \rightarrow \begin{pmatrix} \frac{\partial x u}{y} \\ \frac{\partial y u}{x} \end{pmatrix} \tag{7.20}$$

To find the associated stiffness matrix $\tilde{C}^E$ we compute $C^E \epsilon(u)$ and obtain

$$\begin{align*}
(C^E \epsilon(u))_{11} &= C^E_{1111} \partial x u + C^E_{1122} \partial y v + \frac{C^E_{1112} + C^E_{1121}}{2} (\partial y u + \partial x v) \\
(C^E \epsilon(u))_{12} &= C^E_{1211} \partial x u + C^E_{1222} \partial y v + \frac{C^E_{1212} + C^E_{1221}}{2} (\partial y u + \partial x v) \\
(C^E \epsilon(u))_{21} &= C^E_{2111} \partial x u + C^E_{2122} \partial y v + \frac{C^E_{2112} + C^E_{2121}}{2} (\partial y u + \partial x v) \\
(C^E \epsilon(u))_{22} &= C^E_{2211} \partial x u + C^E_{2222} \partial y v + \frac{C^E_{2212} + C^E_{2221}}{2} (\partial y u + \partial x v)
\end{align*} \tag{7.21-7.24}$$

Using (6.335) – (6.338) we can reduce the problem to

$$\tilde{C}^E \epsilon(u) = \begin{pmatrix} C^E_{1111} & C^E_{1122} & C^E_{1211} & C^E_{1222} \\ C^E_{2111} & C^E_{2122} & C^E_{2211} & C^E_{2222} \end{pmatrix} \begin{pmatrix} \frac{\partial x u}{y} \\ \frac{\partial y v}{x} \\ \frac{\partial x u}{y} + \frac{\partial y v}{x} \end{pmatrix} \tag{7.25}$$

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For the stress amplification matrix $\tilde{Q}^i$ where until the end of the subsection $i = 1, 2$ we compute $Q^i\epsilon(\phi)$ and obtain

\[
(Q^i\epsilon(u))_{11} = Q^i_{1111}\partial_xu + Q^i_{1122}\partial_yv + \frac{Q^i_{1112} + Q^i_{1121}}{2}(\partial_yu + \partial_xv) \quad (7.26)
\]
\[
(Q^i\epsilon(u))_{12} = Q^i_{1211}\partial_xu + Q^i_{1222}\partial_yv + \frac{Q^i_{1212} + Q^i_{1221}}{2}(\partial_yu + \partial_xv) \quad (7.27)
\]
\[
(Q^i\epsilon(u))_{21} = Q^i_{2111}\partial_xu + Q^i_{2122}\partial_yv + \frac{Q^i_{2112} + Q^i_{2121}}{2}(\partial_yu + \partial_xv) \quad (7.28)
\]
\[
(Q^i\epsilon(u))_{22} = Q^i_{2211}\partial_xu + Q^i_{2222}\partial_yv + \frac{Q^i_{2212} + Q^i_{2221}}{2}(\partial_yu + \partial_xv). \quad (7.29)
\]

Using (6.340) – (6.349) and symmetrizing the 12 and 21 component we have

\[
\tilde{Q}^i\epsilon(u) = \begin{pmatrix}
Q^i_{1111} & Q^i_{1122} & \frac{Q^i_{1112} + Q^i_{1121}}{2} \\
Q^i_{2111} & Q^i_{2222} & \frac{Q^i_{2212} + Q^i_{2221}}{2} \\
\frac{Q^i_{1112} + Q^i_{1121}}{2} & \frac{Q^i_{2212} + Q^i_{2221}}{2} & \frac{Q^i_{1112} + Q^i_{1121} + Q^i_{2212} + Q^i_{2221}}{4}
\end{pmatrix}
\begin{pmatrix}
\partial_xu \\
\partial_yv \\
\partial_xv + \partial_yu
\end{pmatrix} \quad (7.30)
\]

with

\[
\tilde{Q}_{11}^i = C^i_{1111} + 2C^i_{1211} + C^i_{2211} \quad (7.31)
\]
\[
\tilde{Q}_{12}^i = \tilde{Q}_{21}^i = C^i_{1111}C^i_{1222} + 2C^i_{1211}C^i_{1222} + C^i_{2211}C^i_{2222} \quad (7.32)
\]
\[
\tilde{Q}_{13}^i = \tilde{Q}_{31}^i = C^i_{1111}\left(\frac{C^i_{1112} + C^i_{1121}}{2}\right) + C^i_{1211}(C^i_{1212} + C^i_{1221}) + C^i_{2211}\left(\frac{C^i_{2212} + C^i_{2221}}{2}\right) \quad (7.33)
\]
\[
\tilde{Q}_{22}^i = C^i_{1122} + 2C^i_{1222} + C^i_{2222} \quad (7.34)
\]
\[
\tilde{Q}_{23}^i = \tilde{Q}_{32}^i = C^i_{1122}\left(\frac{C^i_{1112} + C^i_{1121}}{2}\right) + C^i_{1222}(C^i_{1212} + C^i_{1221}) + C^i_{2222}\left(\frac{C^i_{2212} + C^i_{2221}}{2}\right) \quad (7.35)
\]
\[
\tilde{Q}_{33}^i = \frac{(C^i_{1112} + C^i_{1121})^2}{4} + \frac{(C^i_{1212} + C^i_{1221})^2}{2} + \frac{(C^i_{2212} + C^i_{2221})^2}{4} \quad (7.36)
\]

where $\tilde{Q}^i$ is symmetric.

For simplicity we note that in what follows $\sigma$ and $\epsilon$ refer to the vector representation of stress and strain whereas $C^E$ and $Q$ refer to the matrix representation of the effective stiffness tensor and macrostress modulation tensor.

The reformulated, slightly more general problem is now find the displacement $u$ which is the solution of

\[
\begin{cases}
-\text{div} \sigma = f & \text{in } \Omega \\
\sigma = C^E\epsilon(u) & \text{in } \Omega \\
NCE\epsilon(u) = g & \text{at } \Gamma_N \\
u = h & \text{at } \Gamma_D
\end{cases} \quad (7.37)
\]

where $\Gamma_D \cup \Gamma_N = \Gamma$ and $\Gamma_D \cap \Gamma_N = \emptyset$. We have

\[
\epsilon(u) = \begin{pmatrix} \partial_{x_1}u & \partial_{x_2}v & \partial_{x_1}v + \partial_{x_2}u \end{pmatrix}^T \quad (7.38)
\]
\[
f = (f^1, f^2)^T \quad (7.39)
\]
\[
g = (g^1, g^2)^T \quad (7.40)
\]
\[
h = (h^1, h^2)^T \quad (7.41)
\]
\[
N = \begin{pmatrix} n_1 & 0 & n_2 \\
0 & n_2 & n_1 \end{pmatrix}. \quad (7.42)
\]

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Furthermore, we note that the divergence of $\sigma$ is defined as

$$
div \sigma = \begin{pmatrix} \partial_{x_1} & 0 & \partial_{x_2} \\ 0 & \partial_{x_2} & \partial_{x_1} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{pmatrix}.
$$

(7.43)

### 7.1.3 The Vector-valued Case of Plane Strain

Considering the problem (7.37). Multiplying the PDE in (7.37) with test functions $w^1$ and $w^2$ and integrating over the domain $\Omega$ gives

$$
- \int_\Omega \left\{ w^1(\partial_{x_1}\sigma_{11} + \partial_{x_2}\sigma_{12}) \right\} \, dx = \int_\Omega \left\{ f^1 w^1 \right\} \, dx
$$

(7.44)

Using integration by parts on the left hand side we obtain

$$
\int_\Omega \left\{ \partial_{x_1} w^1 + \partial_{x_2} w^2 \right\} \, dx - \int_\Gamma \left\{ (\sigma_{11}n_1 + \sigma_{12}n_2)w^1 \right\} \, ds = \int_\Omega \left\{ f^1 w^1 \right\} \, dx
$$

(7.45)

Replacing the boundary integral with the Neumann boundary condition from (7.37) leads to

$$
\int_\Omega \left( \begin{array}{cc} \partial_{x_1} w^1 & 0 \\ 0 & \partial_{x_2} w^2 \end{array} \right) \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{pmatrix} \, dx = \int_\Omega \left\{ f^1 w^1 \right\} \, dx + \int_\Gamma \left\{ g^1 w^1 \right\} \, ds
$$

(7.46)

and

$$
\int_\Omega \left( \begin{array}{cc} \partial_{x_1} w^1 & 0 \\ 0 & \partial_{x_2} w^2 \end{array} \right) \begin{pmatrix} \partial_{x_1} u_h \\ \partial_{x_2} v \end{pmatrix} \, dx = \int_\Omega \left\{ f^1 w^1 \right\} \, dx + \int_\Gamma \left\{ g^1 w^1 \right\} \, ds.
$$

(7.47)

In the finite dimensional approximation space we have

$$
\sum_i \int_{\Omega_i} \left( \begin{array}{cc} \partial_{x_1} w^1_h & 0 \\ 0 & \partial_{x_2} w^2_h \end{array} \right) \begin{pmatrix} \partial_{x_1} u_h \\ \partial_{x_2} v_h \end{pmatrix} \, dx = \sum_j \int_{\Gamma_j} \left\{ \frac{f^1 w^1_h}{\mu} \frac{f^2 w^2_h}{\mu} \right\} \, dx + \sum_j \int_{\Gamma_j} \left\{ \frac{g^1 w^1_h}{\mu} \frac{g^2 w^2_h}{\mu} \right\} \, ds.
$$

(7.48)

The displacements $u_h$ and $v_h$ and the test functions $w^1_h$ and $w^2_h$ can be expressed using the same shape functions

$$
u_h = \sum_{i=1}^n u_i H_i \quad v_h = \sum_{i=1}^n v_i H_i
$$

(7.49)

$$
w^1_h = \sum_{i=1}^n H_i \quad w^2_h = \sum_{i=1}^n H_i.
$$

(7.50)

Expressing the strains in (7.48) by shape functions we can write

$$
\begin{pmatrix} \partial_{x_1} u_h \\ \partial_{x_2} v_h \\ \partial_{x_1} v_h + \partial_{x_2} u_h \end{pmatrix} = \begin{pmatrix} \partial_{x_1} H_1 & 0 & \partial_{x_2} H_1 \\ 0 & \partial_{x_2} H_1 & \partial_{x_2} H_2 \end{pmatrix} \begin{pmatrix} \partial_{x_1} H_1 & 0 & \partial_{x_2} H_1 \\ 0 & \partial_{x_2} H_1 & \partial_{x_2} H_2 \end{pmatrix} \begin{pmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ \vdots \\ u_n \\ v_n \end{pmatrix}
$$

(7.51)
with \( \mathbf{\nabla} H_i = \begin{pmatrix} \frac{\partial_x H_i}{\partial x} & 0 \\ 0 & \frac{\partial_y H_i}{\partial y} \\ \frac{\partial_z H_i}{\partial z} & \frac{\partial_y H_i}{\partial z} \end{pmatrix} \) and \( \mathbf{u}_i = \begin{pmatrix} u_i \\ v_i \end{pmatrix} \). With

\[
\begin{pmatrix} \frac{\partial_x W_1}{\partial x} & 0 \\ 0 & \frac{\partial_y W_1}{\partial y} \\ \frac{\partial_z W_1}{\partial z} & \frac{\partial_y W_1}{\partial z} \end{pmatrix} = \begin{pmatrix} \frac{\partial_x u_1}{\partial x} & \frac{\partial_y u_1}{\partial y} \\ 0 & \frac{\partial_x u_2}{\partial x} & \frac{\partial_y u_2}{\partial y} \\ \frac{\partial_x u_3}{\partial x} & \frac{\partial_y u_3}{\partial y} & \frac{\partial_z u_3}{\partial z} \end{pmatrix}
\]

we have at an element domain \( \Omega_i \)

\[
\int_{\Omega_i} \left( \frac{\partial_x W_1}{\partial x} & 0 \\ 0 & \frac{\partial_y W_1}{\partial y} \\ \frac{\partial_z W_1}{\partial z} & \frac{\partial_y W_1}{\partial z} \right) C_h \left( \frac{\partial_x u_1}{\partial x} & \frac{\partial_y u_1}{\partial y} \\ 0 & \frac{\partial_x u_2}{\partial x} & \frac{\partial_y u_2}{\partial y} \\ \frac{\partial_x u_3}{\partial x} & \frac{\partial_y u_3}{\partial y} & \frac{\partial_z u_3}{\partial z} \right) \ dx = \left( \frac{\partial_x H_j}{\partial x} & 0 \\ 0 & \frac{\partial_y H_j}{\partial y} \\ \frac{\partial_z H_j}{\partial z} & \frac{\partial_y H_j}{\partial z} \right) \left( \frac{\partial_x u_1}{\partial x} & \frac{\partial_y u_1}{\partial y} \\ 0 & \frac{\partial_x u_2}{\partial x} & \frac{\partial_y u_2}{\partial y} \\ \frac{\partial_x u_3}{\partial x} & \frac{\partial_y u_3}{\partial y} & \frac{\partial_z u_3}{\partial z} \right)
\]

For the expressions \( \mathbf{\nabla} T H_j C_h \mathbf{\nabla} H_i \) we obtain

\[
\mathbf{\nabla} T H_j C_h \mathbf{\nabla} H_i = \begin{pmatrix} \frac{\partial_x H_j}{\partial x} & 0 & \frac{\partial_y H_j}{\partial y} \\ 0 & \frac{\partial_y H_j}{\partial y} & \frac{\partial_z H_j}{\partial z} \end{pmatrix} C_h \begin{pmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{pmatrix} \begin{pmatrix} \frac{\partial_x H_i}{\partial x} & 0 \\ 0 & \frac{\partial_y H_i}{\partial y} \\ \frac{\partial_z H_i}{\partial z} & \frac{\partial_y H_i}{\partial z} \end{pmatrix}
\]

The forcing term at an element domain \( \Omega_i \) can be written as

\[
\int_{\Omega_i} \left\{ f_i^1 W_1^1 \ f_i^2 W_1^2 \right\} \ dx = \int_{\Omega_i} f_i^1 H_1 \ f_i^2 H_1 \cdots f_i^1 H_n \ f_i^2 H_n \right\}^T \ dx
\]

\[
= (f_i^1 \int_{\Omega_i} H_1 \ dx \ f_i^2 \int_{\Omega_i} H_1 \ dx \cdots f_i^1 \int_{\Omega_i} H_n \ dx \ f_i^2 \int_{\Omega_i} H_n \ dx )^T.
\]
where \( m \) represents the number of boundary points of the finite element of degree of freedom \( n \). The remarks at the end of section 7.1.1 hold for the plane strain problem in a similar way.

### 7.1.4 Reference Elements

![Physical triangle and reference triangle](image)

FIGURE 7.1. Physical triangle and reference triangle.

In a triangular mesh usually each triangle is different from the others. It is therefore convenient to transform the triangle to a reference triangle and do all the computations there. We call the natural coordinates \((\xi, \eta)\) and the physical coordinates \((x, y)\). If in both elements the nodes are numbered clockwise or counterclockwise we obtain

\[
\begin{pmatrix}
x
y
\end{pmatrix} = \begin{pmatrix}
x_2 - x_1 & x_3 - x_1 \\
y_2 - y_1 & y_3 - y_1
\end{pmatrix} \begin{pmatrix}
\xi \\
\eta
\end{pmatrix} + \begin{pmatrix}
x_1 \\
y_1
\end{pmatrix} = J^T \begin{pmatrix}
\xi \\
\eta
\end{pmatrix} + \begin{pmatrix}
x_1 \\
y_1
\end{pmatrix}.
\]

(7.62)

Note that

\[
|J^T| = (x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1) = 2A_\Delta
\]

(7.63)

with \( A_\Delta \) the area of the triangle in the physical domain. We also have that

\[
\begin{pmatrix}
\xi \\
\eta
\end{pmatrix} = \frac{1}{2A_\Delta} \begin{pmatrix}
y_3 - y_1 \\
-(y_2 - y_1)
\end{pmatrix} \begin{pmatrix}
x_2 - x_1 \\
x_3 - x_1
\end{pmatrix} \begin{pmatrix}
x \\
y
\end{pmatrix} - \begin{pmatrix}
x_1 \\
y_1
\end{pmatrix} = J^{-T} \begin{pmatrix}
x \\
y
\end{pmatrix} - \begin{pmatrix}
x_1 \\
y_1
\end{pmatrix}.
\]

(7.64)

For the derivatives we obtain using the chain rule

\[
\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial x} \quad \frac{\partial}{\partial y} = \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial y}
\]

(7.65)

\[
\frac{\partial}{\partial \xi} = \frac{\partial}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial}{\partial y} \frac{\partial y}{\partial \xi} \quad \frac{\partial}{\partial \eta} = \frac{\partial}{\partial x} \frac{\partial x}{\partial \eta} + \frac{\partial}{\partial y} \frac{\partial y}{\partial \eta}
\]

(7.66)

Rewriting these in matrix form and using (7.62) and (7.64) to compute \( \frac{\partial y}{\partial x}, \ldots \) provides

\[
\begin{pmatrix}
\frac{\partial \xi}{\partial y} \\
\frac{\partial \eta}{\partial y}
\end{pmatrix} = \frac{1}{2A_\Delta} \begin{pmatrix}
y_3 - x_1 \\
-(y_2 - y_1)
\end{pmatrix} \begin{pmatrix}
x_2 - x_1 \\
x_3 - x_1
\end{pmatrix} \begin{pmatrix}
\frac{\partial \xi}{\partial \eta} \\
\frac{\partial \eta}{\partial \eta}
\end{pmatrix} = J^{-1} \begin{pmatrix}
\frac{\partial \xi}{\partial \eta} \\
\frac{\partial \eta}{\partial \eta}
\end{pmatrix}
\]

(7.67)

\[
\begin{pmatrix}
\frac{\partial \xi}{\partial \eta} \\
\frac{\partial \eta}{\partial \eta}
\end{pmatrix} = \begin{pmatrix}
x_2 - x_1 & y_2 - y_1 \\
x_3 - x_1 & y_3 - y_1
\end{pmatrix} \begin{pmatrix}
\frac{\partial \xi}{\partial y} \\
\frac{\partial \eta}{\partial y}
\end{pmatrix} = J \begin{pmatrix}
\frac{\partial \xi}{\partial y} \\
\frac{\partial \eta}{\partial y}
\end{pmatrix}
\]

(7.68)

where \( J \) is called the Jacobian matrix for the two-dimensional domain. If in one element the nodes are numbered clockwise and in the other counterclockwise we obtain instead of (7.62), (7.64), (7.67), and
\[
\begin{pmatrix}
  x \\
y
\end{pmatrix}
= \begin{pmatrix}
y_2 - y_1 & y_3 - y_1 \\
x_2 - x_1 & x_3 - x_1
\end{pmatrix}
\begin{pmatrix}
  \xi \\
y_1
\end{pmatrix}
+ \begin{pmatrix}
x_1 \\
y_1
\end{pmatrix}
\]  
\[\tag{7.68}\]

\[
\begin{pmatrix}
  \xi \\
y
\end{pmatrix}
= \frac{1}{2A_b} \begin{pmatrix}
x_3 & -(y_3 - y_1) \\
-(x_2 - x_1) & y_2 - y_1
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}
- \begin{pmatrix}
x_1 \\
y_1
\end{pmatrix}
\]  
\[\tag{7.69}\]

\[
\frac{\partial}{\partial \xi} = \frac{1}{2A_b} \begin{pmatrix}
x_3 & -(y_3 - y_1) \\
-(x_2 - x_1) & y_2 - y_1
\end{pmatrix}
\frac{\partial}{\partial \xi}
\]  
\[\tag{7.70}\]

\[
\frac{\partial}{\partial \eta} = \begin{pmatrix}
y_2 - y_1 & x_2 - x_1 \\
y_3 - y_1 & x_3 - x_1
\end{pmatrix}
\frac{\partial}{\partial \eta}
\]  
\[\tag{7.71}\]

For rectangular elements we want to consider only the case of squares. So in the meshes all elements have the same shape and the same size. We call the length of a side of a square \(s\). The transformation from physical to natural coordinates is then given by

\[
\begin{pmatrix}
x \\
y
\end{pmatrix}
= \begin{pmatrix}
s & 0 \\
0 & s
\end{pmatrix}
\begin{pmatrix}
\xi \\
y
\end{pmatrix}
\quad \begin{pmatrix}
\xi \\
y
\end{pmatrix}
= \begin{pmatrix}
\frac{1}{s} & 0 \\
0 & \frac{1}{s}
\end{pmatrix}
\begin{pmatrix}
x \\
y
\end{pmatrix}
\]  
\[\tag{7.72}\]

For the derivatives we obtain using formulas (7.65)--(7.66)

\[
\begin{pmatrix}
\frac{\partial}{\partial x} & \frac{\partial}{\partial y}
\end{pmatrix}
= \begin{pmatrix}
\frac{1}{s} & 0 \\
0 & \frac{1}{s}
\end{pmatrix}
\begin{pmatrix}
\frac{\partial}{\partial \xi} & \frac{\partial}{\partial \eta}
\end{pmatrix}
= \begin{pmatrix}
s & 0 \\
0 & s
\end{pmatrix}
\begin{pmatrix}
\frac{\partial}{\partial \xi} & \frac{\partial}{\partial \eta}
\end{pmatrix}
\]  
\[\tag{7.73}\]

\[\tag{7.74}\]

### 7.1.5 Shape Functions

In general, the reference triangle with shape functions of order \(k\) has \(\frac{1}{2}(k+1)(k+2)\) degrees of freedom (or nodes). The nodes are given as

\[
P_{ij} = (\xi_i, \eta_j), \quad \text{with} \quad \xi_i = \frac{i-1}{k}, \eta_j = \frac{j-1}{k}, \ i, j = 1 \ldots k+1, \ i+j \leq k+1.
\]  
\[\tag{7.75}\]

The shape functions over the reference triangle are given by

\[
H_{ij}(\xi, \eta) = c \prod_{\substack{i_1, i_2, i_3 \in \{1, 2, 3\} \mid i_1 + i_2 + i_3 = k}} (\xi - \frac{i_1-1}{k})(\eta - \frac{i_2-1}{k})(\frac{i_3-1}{k} - \xi - \eta)
\]  
\[\tag{7.76}\]

\[81\]
where \( i_1, i_2, i_3 \) and \( c \) have to be chosen in a way that \( H_{ij}(\xi_l, \eta_m) = \delta_{il}\delta_{jm} \).

In general, the reference rectangle with shape functions of order \( k \) has \((k + 1)^2\) degrees of freedom (or nodes). The nodes are given as

\[
P_{ij} = (\xi_i, \eta_j), \quad \text{with} \quad \xi_i = \frac{i - 1}{k}, \quad \eta_j = \frac{j - 1}{k}, \quad i, j = 1 \ldots k + 1.
\]  

(7.77)

The shape functions over the reference rectangle are given by

\[
H_{ij}(\xi, \eta) = c \prod_{l=1, m=1 \atop l \neq i, m \neq j}^k (\xi - \frac{l - 1}{k})(\eta - \frac{m - 1}{k}).
\]  

(7.78)

and \( c \) is a constant which has to be chosen such that \( H_{ij}(\xi_i, \eta_j) = 1 \).

**Triangular elements**

![Figure 7.3: Nodes and numbering at the reference triangle for shape functions of order \( k = 1, 2, 3 \).](image)

The linear shape functions of the triangular element in terms of the reference coordinate system are given by

\[
H_1(\xi, \eta) = 1 - \xi - \eta \]  

(7.79)

\[
H_2(\xi, \eta) = \xi \]  

(7.80)

\[
H_3(\xi, \eta) = \eta. \]  

(7.81)

For the derivatives of these functions we easily obtain

\[
\frac{\partial H_1}{\partial \xi} = -1 \quad \frac{\partial H_1}{\partial \eta} = -1 \]  

(7.82)

\[
\frac{\partial H_2}{\partial \xi} = 1 \quad \frac{\partial H_2}{\partial \eta} = 0 \]  

(7.83)

\[
\frac{\partial H_3}{\partial \xi} = 0 \quad \frac{\partial H_3}{\partial \eta} = 1. \]  

(7.84)

The quadratic shape functions of the triangular element in terms of the reference coordinate system are given by

\[
H_1(\xi, \eta) = (1 - \xi - \eta)(1 - 2\xi - 2\eta) \]  

(7.85)

\[
H_2(\xi, \eta) = \xi(2\xi - 1) \]  

(7.86)

\[
H_3(\xi, \eta) = \eta(2\eta - 1) \]  

(7.87)
\[ H_4(\xi, \eta) = 4\xi(1 - \xi - \eta) \quad (7.88) \]
\[ H_5(\xi, \eta) = 4\eta(1 - \xi - \eta) \quad (7.89) \]
\[ H_6(\xi, \eta) = 4\xi\eta \quad (7.90) \]

For the derivatives we get
\[ \frac{\partial H_1}{\partial \xi} = 4(\xi + \eta) - 3 \quad \frac{\partial H_1}{\partial \eta} = 4(\xi + \eta) - 3 \quad (7.91) \]
\[ \frac{\partial H_2}{\partial \xi} = 4\xi - 1 \quad \frac{\partial H_2}{\partial \eta} = 0 \quad (7.92) \]
\[ \frac{\partial H_3}{\partial \xi} = 0 \quad \frac{\partial H_3}{\partial \eta} = 4\eta - 1 \quad (7.93) \]
\[ \frac{\partial H_4}{\partial \xi} = 4(1 - 2\xi - \eta) \quad \frac{\partial H_4}{\partial \eta} = -4\xi \quad (7.94) \]
\[ \frac{\partial H_5}{\partial \xi} = -4\eta \quad \frac{\partial H_5}{\partial \eta} = 4(1 - 2\eta - \xi) \quad (7.95) \]
\[ \frac{\partial H_6}{\partial \xi} = 4\eta \quad \frac{\partial H_6}{\partial \eta} = 4\xi \quad (7.96) \]

The cubic shape functions of the triangular element in terms of the reference coordinate system are given by
\[ H_1(\xi, \eta) = \frac{1}{2}(1 - \xi - \eta)(1 - 3\xi - 3\eta)(2 - 3\xi - 3\eta) \quad (7.97) \]
\[ H_2(\xi, \eta) = \frac{1}{2}\xi(3\xi - 1)(3\xi - 2) \quad (7.98) \]
\[ H_3(\xi, \eta) = \frac{1}{2}\eta(3\eta - 1)(3\eta - 2) \quad (7.99) \]
\[ H_4(\xi, \eta) = \frac{9}{2}\xi(1 - \xi - \eta)(2 - 3\xi - 3\eta) \quad (7.100) \]
\[ H_5(\xi, \eta) = \frac{9}{2}\xi(1 - \xi - \eta)(3\xi - 1) \quad (7.101) \]
\[ H_6(\xi, \eta) = \frac{9}{2}\xi\eta(3\xi - 1) \quad (7.102) \]
\[ H_7(\xi, \eta) = \frac{9}{2}\xi\eta(3\eta - 1) \quad (7.103) \]
\[ H_8(\xi, \eta) = \frac{9}{2}\eta(1 - \xi - \eta)(2 - 3\xi - 3\eta) \quad (7.104) \]
\[ H_9(\xi, \eta) = \frac{9}{2}\eta(1 - \xi - \eta)(3\eta - 1) \quad (7.105) \]
\[ H_{10}(\xi, \eta) = 27\xi\eta(1 - \xi - \eta) \quad (7.106) \]

For the derivatives we get
\[ \frac{\partial H_1}{\partial \xi} = -\frac{1}{2}(1 - 3\xi - 3\eta)(2 - 3\xi - 3\eta) - \frac{3}{2}(1 - \xi - \eta)(2 - 3\xi - 3\eta) - \frac{3}{2}(1 - \xi - \eta)(1 - 3\xi - 3\eta) \quad (7.107) \]
\[
\frac{\partial H_1}{\partial \eta} = -\frac{1}{2}(1-3\xi-3\eta)(2-3\xi-3\eta) - \frac{3}{2}(1-\xi-\eta)(2-3\xi-3\eta) - \frac{3}{2}(1-\xi-\eta)(1-3\xi-3\eta)
\]

(7.109)

\[
\frac{\partial H_1}{\partial \eta} = -\frac{27}{2}\xi^2 - 27\xi\eta - \frac{27}{2}\eta^2 + 18\xi + 18\eta - \frac{11}{2}
\]

(7.108)

\[
\frac{\partial H_2}{\partial \xi} = \frac{1}{2}(3\xi - 1)(3\xi - 2) + \frac{3}{2}\xi(3\xi - 2) + \frac{3}{2}\xi(3\xi - 1)
\]

(7.111)

\[
\frac{\partial H_2}{\partial \eta} = 0
\]

(7.113)

\[
\frac{\partial H_3}{\partial \xi} = 0
\]

(7.114)

\[
\frac{\partial H_3}{\partial \eta} = \frac{1}{2}(3\eta - 1)(3\eta - 2) + \frac{3}{2}\eta(3\eta - 2) + \frac{3}{2}\eta(3\eta - 1)
\]

(7.115)

\[
\frac{\partial H_3}{\partial \eta} = \frac{27}{2}\eta^2 - 9\eta + 1
\]

(7.116)

\[
\frac{\partial H_4}{\partial \xi} = \frac{9}{2}(1 - \xi - \eta)(2 - 3\xi - 3\eta) - \frac{9}{2}\xi(2 - 3\xi - 3\eta) - \frac{27}{2}\xi(1 - \xi - \eta)
\]

(7.117)

\[
\frac{\partial H_4}{\partial \xi} = 9 - 45\xi - \frac{45}{2}\eta + \frac{81}{2}\xi^2 + 54\xi\eta + \frac{27}{2}\eta^2
\]

(7.118)

\[
\frac{\partial H_4}{\partial \eta} = -\frac{9}{2}\xi(2 - 3\xi - 3\eta) - \frac{27}{2}\xi(1 - \xi - \eta)
\]

(7.119)

\[
\frac{\partial H_5}{\partial \xi} = \frac{9}{2}(1 - \xi - \eta)(3\xi - 1) - \frac{9}{2}\xi(3\xi - 1) + \frac{27}{2}\xi(1 - \xi - \eta)
\]

(7.121)

\[
\frac{\partial H_5}{\partial \xi} = -\frac{81}{2}\xi^2 - 27\xi\eta + 36\xi + \frac{9}{2}\eta - \frac{9}{2}
\]

(7.122)

\[
\frac{\partial H_6}{\partial \eta} = -\frac{9}{2}\xi(3\xi - 1)
\]

(7.123)

\[
\frac{\partial H_6}{\partial \xi} = \frac{9}{2}\eta(3\xi - 1) + \frac{27}{2}\xi\eta = 27\xi\eta - \frac{9}{2}\eta
\]

(7.124)

\[
\frac{\partial H_6}{\partial \eta} = \frac{9}{2}\xi(3\xi - 1)
\]

(7.125)

\[
\frac{\partial H_7}{\partial \xi} = \frac{9}{2}\eta(3\eta - 1)
\]

(7.126)

\[
\frac{\partial H_7}{\partial \eta} = \frac{9}{2}(3\eta - 1) + \frac{27}{2}\xi\eta = 27\xi\eta - \frac{9}{2}\xi
\]

(7.127)
\[
\frac{\partial H_8}{\partial \xi} = -\frac{9}{2} \eta (3\eta - 1) \quad (7.128)
\]
\[
\frac{\partial H_8}{\partial \eta} = \frac{9}{2} (1 - \xi - \eta)(3\eta - 1) - \frac{9}{2} \eta (3\eta - 1) \frac{27}{2} \eta (1 - \xi - \eta) \quad (7.129)
\]
\[
= -27\xi \eta - \frac{81}{2} \eta^2 + \frac{9}{2} \xi + 36\eta - \frac{9}{2} \quad (7.130)
\]
\[
\frac{\partial H_9}{\partial \xi} = -\frac{9}{2} \eta (2 - 3\xi - 3\eta) - \frac{27}{2} \eta (1 - \xi - \eta) = 27\eta^2 + 27\xi \eta - \frac{45}{2} \eta \quad (7.131)
\]
\[
\frac{\partial H_9}{\partial \eta} = \frac{9}{2} (1 - \xi - \eta)(2 - 3\xi - 3\eta) - \frac{9}{2} \eta (2 - 3\xi - 3\eta) - \frac{27}{2} \eta (1 - \xi - \eta) \quad (7.132)
\]
\[
= \frac{27}{2} \xi^2 + 54\xi \eta + \frac{81}{2} \eta^2 - \frac{45}{2} \xi - 45\eta + 9 \quad (7.133)
\]
\[
\frac{\partial H_{10}}{\partial \xi} = 27\eta (1 - \xi - \eta) - 27\xi \eta = -27\eta^2 - 54\xi \eta + 27\eta \quad (7.134)
\]
\[
\frac{\partial H_{10}}{\partial \eta} = 27\xi (1 - \xi - \eta) - 27\xi \eta = -27\xi^2 - 54\xi \eta + 27\xi \quad (7.135)
\]

**Rectangular elements**

![Rectangular elements](https://via.placeholder.com/150)

**FIGURE 7.4.** Nodes and numbering at the reference rectangle for shape functions of order \(k = 1, 2, 3\).

For rectangular elements the linear shape functions in terms of the reference coordinate system are given by

\[
H_1(\xi, \eta) = \eta (1 - \xi) \quad (7.136)
\]
\[
H_2(\xi, \eta) = \xi \eta \quad (7.137)
\]
\[
H_3(\xi, \eta) = \xi \eta - \xi - \eta + 1 \quad (7.138)
\]
\[
H_4(\xi, \eta) = \xi (1 - \eta) \quad (7.139)
\]

The quadratic shape functions of the rectangular element are given by

\[
H_1(\xi, \eta) = (1 - \xi)(1 - 2\xi)\eta(2\eta - 1) \quad (7.140)
\]
\[
H_2(\xi, \eta) = \xi (2\xi - 1)\eta(2\eta - 1) \quad (7.141)
\]
\[
H_3(\xi, \eta) = \xi (2\xi - 1)(1 - \eta)(1 - 2\eta) \quad (7.142)
\]
\[
H_4(\xi, \eta) = (1 - \xi)(1 - 2\xi)(1 - \eta)(1 - 2\eta) \quad (7.143)
\]
7.1.6 The Case of Linear Shape Functions

For linear shape functions one can besides the general way of working with a reference element proceed directly. To find the shape functions of each triangle which are of the form \( H_i = a_i x + b_i y + c_i, \ i = 1, 2, 3 \)
we have to consider that the function $H_i$ equals 1 at $P_i$ and 0 at the other two points. So we have to solve 3 systems of linear equations

\[
\begin{align*}
    a_i x_1 + b_i y_1 + c_i &= \delta_1, \\
    a_i x_2 + b_i y_2 + c_i &= \delta_2, \\
    a_i x_3 + b_i y_3 + c_i &= \delta_3.
\end{align*}
\]  

(7.165)

We have that

\[
\begin{vmatrix}
    x_1 & y_1 & 1 \\
    x_2 & y_2 & 1 \\
    x_3 & y_3 & 1
\end{vmatrix} = \begin{vmatrix}
    x_2 - x_1 & y_2 - y_1 \\
    x_3 - x_1 & y_3 - y_1
\end{vmatrix} = 2 A_{\Delta}
\]  

(7.166)

where $A_{\Delta}$ is the area of the triangle. Using Cramer’s rule to solve (7.165) we obtain for $a_i, b_i$ and $c_i, i = 1, 2, 3$

\[
\begin{align*}
    a_1 &= \frac{y_2 - y_3}{2 A_{\Delta}}, & b_1 &= \frac{x_3 - x_2}{2 A_{\Delta}}, & c_1 &= \frac{x_2 y_3 - y_2 x_3}{2 A_{\Delta}}, \\
    a_2 &= \frac{x_1 - x_3}{2 A_{\Delta}}, & b_2 &= \frac{x_1 y_3 - y_1 x_3}{2 A_{\Delta}}, & c_2 &= \frac{x_1 y_3 - y_1 x_3}{2 A_{\Delta}}, \\
    a_3 &= \frac{y_1 - y_2}{2 A_{\Delta}}, & b_3 &= \frac{x_3 y_1 - y_3 x_1}{2 A_{\Delta}}, & c_3 &= \frac{x_1 y_3 - y_1 x_3}{2 A_{\Delta}}.
\end{align*}
\]  

(7.167)

For the derivatives of the shape functions we obtain $\partial_x H_i = a_i$, $\partial_y H_i = b_i$. In the next sections we have to compute integrals of the following type

\[
\int_{\Delta} \partial_x H_i dx = a_i A_{\Delta} \quad \int_{\Delta} \partial_y H_i dx = b_i A_{\Delta}
\]  

(7.168)

\[
\int_{\Delta} H_i dx = \frac{1}{3} A_{\Delta}
\]  

(7.169)

\[
\int_{P_i} H_i ds = \frac{1}{2} \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}
\]  

(7.170)

For boundary integrals we obtain over a triangle

\[
\int_{(x_i,y_i)}^{(x_j,y_j)} g(x,y) ds = \frac{1}{l} \int_{(\xi_i,\eta_i)}^{(\xi_j,\eta_j)} g(\xi,\eta) ds
\]  

(7.171)

with $l = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$.

For the linear shape functions of the rectangular element we get for the derivatives

\[
\begin{align*}
    \frac{\partial H_1}{\partial \xi} &= -\eta, & \frac{\partial H_1}{\partial \eta} &= 1 - \xi, \\
    \frac{\partial H_2}{\partial \xi} &= \eta, & \frac{\partial H_2}{\partial \eta} &= \xi, \\
    \frac{\partial H_3}{\partial \xi} &= \eta - 1, & \frac{\partial H_3}{\partial \eta} &= \xi - 1, \\
    \frac{\partial H_4}{\partial \xi} &= 1 - \eta, & \frac{\partial H_4}{\partial \eta} &= -\xi.
\end{align*}
\]  

(7.172) - (7.175)
Using transformation (7.74) we have for the derivatives of the physical element

\[
\frac{\partial H_1}{\partial x} = \frac{\partial H_1}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial H_1}{\partial \eta} \frac{\partial \eta}{\partial x} = -\frac{\eta}{s} \quad \frac{\partial H_1}{\partial y} = \frac{\partial H_1}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial H_1}{\partial \eta} \frac{\partial \eta}{\partial y} = -\frac{1}{s} \xi \quad (7.176)
\]

\[
\frac{\partial H_2}{\partial x} = \frac{\partial H_2}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial H_2}{\partial \eta} \frac{\partial \eta}{\partial x} = \frac{\eta}{s} \quad \frac{\partial H_2}{\partial y} = \frac{\partial H_2}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial H_2}{\partial \eta} \frac{\partial \eta}{\partial y} = \frac{\xi}{s} \quad (7.177)
\]

\[
\frac{\partial H_3}{\partial x} = \frac{\partial H_3}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial H_3}{\partial \eta} \frac{\partial \eta}{\partial x} = \frac{\eta - 1}{s} \quad \frac{\partial H_3}{\partial y} = \frac{\partial H_3}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial H_3}{\partial \eta} \frac{\partial \eta}{\partial y} = \frac{\xi - 1}{s} \quad (7.178)
\]

\[
\frac{\partial H_4}{\partial x} = \frac{\partial H_4}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial H_4}{\partial \eta} \frac{\partial \eta}{\partial x} = \frac{1 - \eta}{s} \quad \frac{\partial H_4}{\partial y} = \frac{\partial H_4}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial H_4}{\partial \eta} \frac{\partial \eta}{\partial y} = \frac{\eta}{s} \quad (7.179)
\]

As shown in the sections above one has to compute integrals of the form \(\int_0^s \int_0^s \frac{\partial H_i}{\partial x} \frac{\partial H_j}{\partial x} \, dx \, dy\) which turn out to be the same as the integrals \(\int_0^1 \int_0^1 \frac{\partial H_i}{\partial x} \frac{\partial H_j}{\partial x} \, d\xi \, d\eta\) so that all the integration can be done on the reference element. Thus we obtain for the following integrals

\[
\pm \int_0^1 \int_0^1 \xi^2 \, d\xi \, d\eta = \pm \int_0^1 \int_0^1 \eta^2 \, d\xi \, d\eta = \pm \int_0^1 \frac{1}{3} \, d\eta = \pm \frac{1}{3} \quad (7.180)
\]

\[
\pm \int_0^1 \int_0^1 (\xi - 1)^2 \, d\xi \, d\eta = \pm \int_0^1 \int_0^1 (\eta - 1)^2 \, d\xi \, d\eta = \pm \int_0^1 \frac{1}{3} \, d\eta = \pm \frac{1}{3} \quad (7.181)
\]

\[
\pm \int_0^1 \int_0^1 \xi \eta \, d\xi \, d\eta = \pm \int_0^1 \frac{1}{2} \eta \, d\eta = \pm \frac{1}{4} \quad (7.182)
\]

\[
\pm \int_0^1 \int_0^1 (\xi - 1)(\eta - 1) \, d\xi \, d\eta = \pm \int_0^1 \frac{1}{2}(\eta - 1) \, d\eta = \pm \frac{1}{4} \quad (7.183)
\]

\[
\pm \int_0^1 \int_0^1 \xi(\xi - 1) \, d\xi \, d\eta = \pm \int_0^1 \int_0^1 \eta(\eta - 1) \, d\xi \, d\eta = \pm \int_0^1 \frac{1}{6} \, d\eta = \pm \frac{1}{6} \quad (7.184)
\]

\[
\pm \int_0^1 \int_0^1 \xi(\eta - 1) \, d\xi \, d\eta = \pm \int_0^1 \int_0^1 \eta(\xi - 1) \, d\xi \, d\eta = \pm \int_0^1 \frac{1}{2}(\eta - 1) \, d\eta = \pm \frac{1}{4} \quad (7.185)
\]

and we can arrange an integration table

\[
\begin{array}{cccccccc}
\frac{\partial H_1}{\partial x} & \frac{\partial H_1}{\partial y} & \frac{\partial H_2}{\partial x} & \frac{\partial H_2}{\partial y} & \frac{\partial H_3}{\partial x} & \frac{\partial H_3}{\partial y} & \frac{\partial H_4}{\partial x} & \frac{\partial H_4}{\partial y} \\
\frac{1}{3} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{6} & -\frac{1}{4} & -\frac{1}{3} & -\frac{1}{6} \\
-\frac{1}{4} & \frac{1}{3} & 1 & 1 & -\frac{1}{4} & -\frac{1}{3} & 1 & -\frac{1}{6} \\
-\frac{1}{3} & \frac{1}{4} & \frac{1}{3} & -\frac{1}{4} & -\frac{1}{3} & 1 & -\frac{1}{6} & \frac{1}{4} \\
-\frac{1}{4} & \frac{1}{6} & \frac{1}{4} & \frac{1}{3} & -\frac{1}{6} & 1 & -\frac{1}{3} & \frac{1}{6} \\
-\frac{1}{6} & \frac{1}{4} & \frac{1}{6} & \frac{1}{3} & -\frac{1}{6} & 1 & -\frac{1}{3} & \frac{1}{6} \\
-\frac{1}{4} & \frac{1}{6} & \frac{1}{4} & \frac{1}{3} & -\frac{1}{6} & 1 & -\frac{1}{3} & \frac{1}{6} \\
-\frac{1}{6} & \frac{1}{4} & \frac{1}{6} & \frac{1}{3} & -\frac{1}{6} & 1 & -\frac{1}{3} & \frac{1}{6} \\
\end{array} \quad (7.186)
\]

In case of linear elasticity we obtain for the expressions \(\nabla^T H_j C^i \nabla H_i\)

\[
\nabla^T H_j C^i \nabla H_i = \left( \begin{array}{ccc}
\partial_x H_j & 0 & \partial_y H_j \\
0 & \partial_y H_j & \partial_z H_j \\
\end{array} \right) \left( \begin{array}{ccc}
C_{11}^i & C_{12}^i & C_{13}^i \\
C_{12}^i & C_{22}^i & C_{23}^i \\
C_{13}^i & C_{23}^i & C_{33}^i \\
\end{array} \right) \left( \begin{array}{ccc}
\partial_x H_i & 0 \\
0 & \partial_y H_i \\
\end{array} \right) \quad (7.187)
\]
For the local stiffness matrix we get by using table (7.186)

\[
\begin{pmatrix}
C_{11} & C_{13} & C_{15} \\
C_{13} & C_{12} & C_{14} \\
C_{15} & C_{14} & C_{16}
\end{pmatrix}
\]

(7.188)

with

\[
K^l = \begin{pmatrix}
K_{11}^l & K_{12}^l \\
K_{12}^l & K_{22}^l
\end{pmatrix}
\]

(7.190)

\[
K_{11}^l = \begin{pmatrix}
\frac{C_{11}}{3} & \frac{C_{13}}{3} & \frac{C_{15}}{3} \\
\frac{C_{13}}{3} & \frac{C_{12}}{3} & \frac{C_{14}}{3} \\
\frac{C_{15}}{3} & \frac{C_{14}}{3} & \frac{C_{16}}{3}
\end{pmatrix}
\]

(7.191)

\[
K_{22}^l = \begin{pmatrix}
\frac{C_{11}}{3} & \frac{C_{13}}{3} & \frac{C_{15}}{3} \\
\frac{C_{13}}{3} & \frac{C_{12}}{3} & \frac{C_{14}}{3} \\
\frac{C_{15}}{3} & \frac{C_{14}}{3} & \frac{C_{16}}{3}
\end{pmatrix}
\]

(7.192)

\[
K_{12}^l = \begin{pmatrix}
\frac{C_{11}}{3} & \frac{C_{13}}{3} & \frac{C_{15}}{3} \\
\frac{C_{13}}{3} & \frac{C_{12}}{3} & \frac{C_{14}}{3} \\
\frac{C_{15}}{3} & \frac{C_{14}}{3} & \frac{C_{16}}{3}
\end{pmatrix}
\]

(7.193)

7.1.7 Gaussian Integration

In the above sections it became necessary to compute integrals of shape functions. A common way to do this numerically is to use Gaussian integration methods. Here integrals of the form

\[
I(f) = \int_a^b w(x)f(x)dx
\]

(7.194)

where \(w(x)\) is a given nonnegative weight function on the interval \([a, b]\) are considered. We want to replace the integral by an integration rule of type

\[
I(f) = \sum_{i=1}^n w_if(x_i).
\]

(7.195)

The abscesses \(x_i\) are not required to form a uniform partition of the interval \([a, b]\). One tries to choose the \(x_i\) and the \(w_i\) to maximize the order of the integration method, i.e. to maximize the degree for which
all polynomials are integrated exactly. This leads to a class of Gaussian integration rules or Gaussian quadrature formulas. These rules are unique and of the order $2n - 1$, $w_i > 0$ and $a < x_i < b$ for $i = 1 \ldots n$. We use the notation
\[ \Pi_j = \{ p | p(x) = x^j + a_{j-1}x^{j-1} + \ldots + a_0 \} \] (7.196)
for the set of real normed polynomials of degree $j$. We define the scalar product
\[ (f, g) = \int_a^b w(x) f(x) g(x) dx \] (7.197)
on the linear space $L^2[a, b]$ of all functions for which the integral
\[ (f, f) = \int_a^b w(x)[f(x)]^2 dx \] (7.198)
is finite. Two functions $f, g \in L^2[a, b]$ are called orthogonal if $(f, g) = 0$. There exists a sequence of orthogonal polynomials, the system of orthogonal polynomials associated with the weight function $w(x)$.

**Theorem 7.1.** There exist polynomials $p_j \in \Pi_j, j = 0, 1, \ldots$, such that
\[ (p_i, p_k) = 0 \text{ for } i \neq k. \] (7.199)
These polynomials are uniquely defined by the recursions
\[ p_{i+1}(x) = (x - \delta_{i+1})p_i(x) - \gamma^2_{i+1}p_{i-1}(x), \quad i \geq 0 \] (7.200)
where $p_0(x) = 1$, $p_{-1}(x) = 0$, and
\[ \delta_{i+1} = \frac{(xp_i, p_i)}{(p_i, p_i)} \quad \text{for} \quad i \geq 0 \] (7.201)
\[ \gamma^2_{i+1} = \begin{cases} 1 & \text{for} \quad i = 0 \\ \frac{(p_i, p_i)}{(p_{i-1}, p_{i-1})} & \text{for} \quad i \geq 1. \end{cases} \] (7.202)

To determine the integration points $x_i$ we use the following theorem

**Theorem 7.2.** Let $x_1, \ldots, x_n$ be the roots of the $n$th orthogonal polynomial $p_n(x)$, and let $w_1, \ldots, w_n$ be the solution of the nonsingular system of equations
\[ \sum_{i=1}^n p_k(x_i)w_i = \begin{cases} (p_0, p_0) & \text{if} \quad k = 0 \\ 0 & \text{if} \quad k = 1, \ldots, n - 1. \end{cases} \] (7.203)
Then $w_i > 0$ for $i = 1, \ldots, n$, and
\[ \int_a^b w(x)f(x)dx = \sum_{i=1}^n w_ip(x_i) \] (7.204)
holds for all polynomials of degree $2n - 1$. The positive numbers $w_i$ are called weights.
It is not possible to find numbers \( x_i, w_i, i = 1, \ldots, n \), such that (7.204) holds for all polynomials of degree \( 2n \).

It remains to find a method for calculating the weights. The theory of orthogonal polynomials is closely connected to the theory of real tridiagonal matrices

\[
J_j = \begin{pmatrix}
\delta_1 & \gamma_2 & & & \\
\gamma_2 & \delta_2 & \ddots & & \\
& \ddots & \ddots & \gamma_j \\
& & \delta_{j-1} & \gamma_j & \delta_j
\end{pmatrix}
\] (7.205)

The characteristic polynomial \( \det(J_j - xI_j) \) of the \( J_j \) satisfies the recursion (7.200) with the matrix elements \( \delta_j, \gamma_j \) as the coefficients. Therefore, \( p_j \) is the characteristic polynomial of the tridiagonal matrix \( J_j \) and we have

**Theorem 7.3.** The roots \( x_i, i = 1, \ldots, n \), of the \( n \)th orthogonal polynomial \( p_n \) are the eigenvalues of the tridiagonal matrix \( J_n \) in (7.205).

With respect to the weights \( w_i \), we have

**Theorem 7.4.** Let \( v^i = (v^i_1, \ldots, v^i_n)^T \) be an eigenvector of \( J_n \) (7.205) for the eigenvalue \( x_i \), \( J_nv^i = x_iv^i \). Suppose \( v^i \) is scaled such that

\[
(v^i)^Tv^i = (p_0, p_0) = \int_a^b w(x)dx.
\] (7.206)

Then the weights are given by

\[
w_i = (v^i_1)^2, i = 1, \ldots, n.
\] (7.207)

For the most common weight function \( w(x) = 1 \) and the interval \([-1, 1]\), the results of theorem 7.2 are due to Gauss. The corresponding orthogonal polynomials are

\[
p_k(x) = \frac{k!}{(2k)!} \frac{d^k}{dx^k}(x^2 - 1)^k, \quad k = 0, 1, \ldots.
\] (7.208)

Up to a factor, the polynomials (7.208) are the Legendre polynomials. The first polynomials are

\[
\begin{align*}
p_0(x) &= 1 \quad (7.209) \\
p_1(x) &= x \quad (7.210) \\
p_2(x) &= x^2 - 3 \quad (7.211) \\
p_3(x) &= x^3 - \frac{3}{5}x \quad (7.212) \\
p_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{35} \quad (7.213) \\
p_5(x) &= x^5 - \frac{10}{9}x^3 + \frac{5}{21}x. \quad (7.214)
\end{align*}
\]

To compute \( \delta_i \) and \( \gamma_i \) we use (7.201) and (7.202). All the polynomials \( p_i \) are either odd or even functions. So the squares of the polynomials are even and \( (xp_i, p_i) = 0 \). Therefore we have that \( \delta_i = 0 \). For \( (p_i, p_i) \)
and $\gamma_i$ we obtain

\[
(p_0, p_0) = 2
\]

\[
(p_1, p_1) = \frac{2}{3}, \quad \gamma_2 = \frac{1}{3}
\]

\[
(p_2, p_2) = \frac{8}{15}, \quad \gamma_3 = \frac{4}{15}
\]  

(7.215)

\[
(p_3, p_3) = \frac{8}{175}, \quad \gamma_4 = \frac{9}{35}
\]

\[
(p_4, p_4) = \frac{128}{11025}, \quad \gamma_5 = \frac{16}{63}
\]

Finding the roots of the polynomials $p_j$ and the the first component of the eigenvectors of $J_j$ we obtain the integration points and weights for this important special case which are given in the table 7.1. Table

<table>
<thead>
<tr>
<th>n</th>
<th>$w_i$</th>
<th>$x_i$</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>$w_1$ 2</td>
<td>$x_1 = 0$</td>
</tr>
<tr>
<td>2</td>
<td>$w_1 = w_2 = 1$</td>
<td>$x_2 = -x_1 = \frac{1}{\sqrt{3}} = 0.577350269189626$</td>
</tr>
<tr>
<td>3</td>
<td>$w_1 = w_3 = \frac{5}{9}$, $w_2 = \frac{8}{9}$</td>
<td>$x_3 = -x_1 = \sqrt{\frac{3}{5}} = 0.774596669241483$</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>$w_1 = w_4 = 0.347854845137454$, $w_2 = w_3 = 0.652145154862546$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$w_1 = w_5 = 0.236926885056189$, $w_2 = w_4 = 0.478628670499366$, $w_3 = \frac{128}{225} = 0.568888888888889$</td>
<td>$x_5 = -x_1 = \frac{1}{21}\sqrt{245 + 14\sqrt{70}} = 0.906179845938664$</td>
</tr>
<tr>
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</tbody>
</table>

7.1 can be also used for integration over the rectangular reference element. Here we have

\[
\int_0^1 \int_0^1 f(\xi, \eta) d\xi d\eta = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \omega_i \omega_j f(\xi_i, \eta_j) \quad (7.216)
\]

where the $\xi_i, \eta_j, \omega_i, \omega_j$ are the transformed values of $x_i, w_i$

\[
\xi_i = \frac{1}{2}(x_i + 1) \quad (7.217)
\]

\[
\omega_i = \frac{w_i}{2} \quad (7.218)
\]

For integration over the triangular reference element table B.1 can be used.
7.2 Iterative Methods for Solving Systems of Linear Equations

The Finite Element Method requires to solve a system of linear equations

\[ Ax = b. \quad (7.219) \]

The matrix \( A \) is symmetric, positive definite, and sparse. Classical elimination methods are not suitable for those systems because they tend to fill in the intermediate matrices in the solution process. A better choice are iterative methods. Here in each iteration step only a matrix vector multiplication is required so that one can save the matrix in a sparse format. In this context we only want to consider Conjugate Gradient methods. For further details on iterative methods see for instance [29], [32], [11].

7.2.1 Conjugate Gradient Method

Let \( A \) be a symmetric, positive definite matrix. Then solving the system (7.219) is equivalent to minimizing the quadratic functional

\[ \phi(w) = \frac{1}{2} (Aw, w) - (b, w). \quad (7.220) \]

The minimum value of \( \phi \) is \(-(1/2)(A^{-1}b, b)\), and is attained for \( x = A^{-1}b \). We notice that the residual defined as

\[ r^k = b - Ax^k \quad (7.221) \]

is the negative gradient of \( \phi \) at \( x^k \)

\[ r^k = -\nabla \phi(x^k). \quad (7.222) \]

The new iterate \( x^{k+1} \) is reached by updating \( x^k \) in a direction \( p^k \)

\[ x^{k+1} = x^k + \alpha_k p^k. \quad (7.223) \]

In the Conjugate Gradient method the directions \( p^k \) are \( A \)-conjugate. They satisfy the orthogonality property \( (p^j, Ap^m) = 0 \) for \( m \neq j \). In particular

\[ (p^{k+1}, Ap^k) = 0, \text{ for all } k \in \mathbb{N}. \quad (7.224) \]

Let \( p^0, \ldots, p^m \) be linearly independent vectors and \( x^0 \) being an initial guess. Then \( x^{k+1} \) in (7.223) minimizes the functional \( \phi \) on the \((k+1)\)-hyperplane

\[ w = x^0 + \sum_{j=1}^k \gamma_j p^j, \quad \gamma_j \in \mathbb{R}, \quad (7.225) \]

if, and only if, \( p^j \) are \( A \)-conjugate and

\[ \alpha_k = \frac{(r^k, p^k)}{(p^k, Ap^k)}. \quad (7.226) \]

Therefore the conjugate gradient method can be formulated in the following way. Let \( x^0 \) be an initial guess, \( r^0 = b - Ax^0 \), and set \( p^0 = r^0 \). For each \( k \in \mathbb{N} \), the \( k \)-th iteration is made according to

\[ \begin{align*}
\alpha_k &= \frac{(r^k, p^k)}{(p^k, Ap^k)} = \frac{|r^k|^2}{(p^k, Ap^k)} \quad (7.227) \\
x^{k+1} &= x^k + \alpha_k p^k \quad (7.228) \\
r^{k+1} &= r^k - \alpha_k Ap^k \quad (7.229) \\
\beta_{k+1} &= -\frac{(r^{k+1}, Ap^k)}{(p^k, Ap^k)} = \frac{|r^{k+1}|^2}{|r^k|^2} \quad (7.230) \\
p^{k+1} &= p^k + \beta_k p^k. \quad (7.231)
\end{align*} \]
A frequently used stopping criterion is
\[
\frac{|r^k|}{|b|} < \varepsilon
\]  
(7.232)
where \( \varepsilon > 0 \) is a prescribed tolerance and usually chosen to be \( \varepsilon = 10^{-6} \).

### 7.2.2 Preconditioning

The performance of an iterative method may strongly benefit from a low condition number of the system matrix. For ill-conditioned systems one can use a preconditioner which means a non-singular matrix \( P \) and consider the equivalent system
\[
P^{-1}Ax = P^{-1}b.
\]  
(7.233)

The basic requirements for \( P \) to be a good preconditioner are

- \( P \) has to be easy to invert.
- The condition number of \( P^{-1}A \) should be significantly smaller than the one of \( A \).

A problem with (7.233) is that \( P^{-1}A \) could fail to be symmetric or positive definite even if both factors are so. However, if both \( P \) and \( A \) are symmetric and positive definite we can apply the conjugate gradient iteration (7.227-7.231) directly to (7.233) by replacing \( A \) with \( P^{-1}A \), \( b \) with \( P^{-1}b \), and \( r^k \) with \( z^k = P^{-1}r^k \). The preconditioned conjugate gradient method is then as follows

\[
\alpha_k = \frac{(z^k, r^k)}{(p^k, Ap^k)}
\]  
(7.234)

\[
x^{k+1} = x^k + \alpha_k p^k
\]  
(7.235)

\[
r^{k+1} = r^k - \alpha_k Ap^k
\]  
(7.236)

\[
Pz^{k+1} = r^{k+1}
\]  
(7.237)

\[
\beta_{k+1} = \frac{(z^{k+1}, r^k)}{(z^k, r^k)}
\]  
(7.238)

\[
p^{k+1} = z^{k+1} + \beta_{k+1} p^k.
\]  
(7.239)

The initialization is accomplished by taking an initial guess \( x^0 \) and setting \( r^0 = b - Ax^0 \), \( p^0 = z^0 = P^{-1}r^0 \).

Now the question is how to choose \( P \) so that \( P^{-1}A \) has an improved condition number. A simple preconditioner is provided by the diagonal matrix
\[
P = \text{diag}(a_{11}, \ldots, a_{nn})
\]  
(7.240)

which is the Jacobi preconditioner, or else by

\[
P = \text{diag}(c_1, \ldots, c_n), \text{ with } c_i = \left( \sum_{j=1}^{n} a_{ij} \right)^{\frac{1}{2}}.
\]  
(7.241)

Another possible procedure is to write the preconditioner \( P \) as
\[
P = HH^T
\]  
(7.242)
where $H$ is a non-singular matrix. One way to achieve this is to represent the matrix $A$ as

$$
A = \begin{pmatrix}
U_A \\
D_A \\
L_A
\end{pmatrix}
$$

(7.243)

where $D_A$ is the diagonal of $A$ and $L_A, U_A$ are its lower and upper triangular parts, respectively, and set

$$
D = \begin{pmatrix}
D_A & 0 \\
0 & D_A
\end{pmatrix} \quad E = \begin{pmatrix}
0 & 0 \\
L_A & 0
\end{pmatrix} \quad F = \begin{pmatrix}
0 & U_A \\
0 & 0
\end{pmatrix}
$$

(7.244)

Then the Symmetric Successive Over-Relaxation (S.S.O.R.) preconditioner is given by

$$
P = \frac{1}{\omega(2-\omega)}(D + \omega E)D^{-1}(D + \omega E)^T
$$

(7.245)

where $0 < \omega < 2$. In this case a matrix $H$ that satisfies $P = HH^T$ is given by

$$
H = \frac{1}{\sqrt{\omega(2-\omega)}}(D + \omega E)(\sqrt{D})^{-1}(D + \omega E)^T, \text{ with } \sqrt{D} = \text{diag}(\sqrt{a_{11}}, \ldots, \sqrt{a_{nn}}).
$$

(7.246)

Table 7.2 shows a comparison of the iterations and time needed until convergence for the conjugate gradient algorithm with and without preconditioning.

| TABLE 7.2. Integration points and weights triangular domains. |
|-----------------|-----------------|-----------------|-----------------|
|                 | without preconditioning | Jacobi preconditioner | S.S.O.R. preconditioner |
| iterations      | 5024             | 2577             | 974             |
| time [s]        | 178              | 83               | 36              |

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References


A. Pictures of the Shape Functions

FIGURE A.1. Linear (left), quadratic (middle) and cubic (right) shape functions for triangular elements.
FIGURE A.2. Linear (left), quadratic (middle) and cubic (right) shape functions for rectangular elements.
### B. Integration Points in Triangles

**TABLE B.1. Integration points and weights for triangular domains.**

<table>
<thead>
<tr>
<th>Int.-order</th>
<th>( \omega_i )</th>
<th>( \xi_i )</th>
<th>( \eta_i )</th>
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<td>( \frac{1}{6} )</td>
<td>( \frac{1}{6} )</td>
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<tr>
<td></td>
<td>( \frac{1}{6} )</td>
<td>( \frac{2}{3} )</td>
<td>( \frac{1}{3} )</td>
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<tr>
<td></td>
<td>( \frac{1}{6} )</td>
<td>( \frac{1}{6} )</td>
<td>( \frac{2}{3} )</td>
</tr>
<tr>
<td>7 points</td>
<td>( \frac{0.0629695902724}{3} )</td>
<td>( \frac{0.1012865073235}{3} )</td>
<td>( \frac{0.1012865073235}{3} )</td>
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<td>( \frac{0.0629695902724}{3} )</td>
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<td>( \frac{0.7974269853531}{3} )</td>
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<td>( \frac{0.0597158717898}{3} )</td>
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<td>( \frac{0.4701420641051}{3} )</td>
<td>( \frac{0.4701420641051}{3} )</td>
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<td>( \frac{0.0597158717898}{3} )</td>
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Vita

Michael Stuebner (Stübner) was born on February 22, 1970, in Zwickau, Saxony (Sachsen), Germany. He finished his undergraduate studies in applied mathematics at the Technical University (Technische Universität) Chemnitz, Germany, in May 1997. After continuing his research in mathematics and material science at the University of Mining (Bergakademie) Freiberg, Germany he came in January 2000 to Louisiana State University to pursue graduate studies in applied mathematics. He earned a master of science degree in mathematics from Louisiana State University in May 2002. He is currently a candidate for the degree of Doctor of Philosophy in mathematics, which will be awarded in August 2006.