Micromechanical Modelling of Composite Materials

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Abstract

This is an intermediate report on the micromechanical modelling of composite materials. The main goal of the investigations is to derive material models for composite materials, which take into account both the microstructure of the composite and the micromechanical properties of its constituents, as well as their interactions. To that end, it is convenient to distinguish three different scales: the microscopic scale of the inhomogeneities, the macroscopic scale of the material body, and an intermediate mesoscopic scale. The latter is much larger than the microscopic and much smaller than the macroscopic scale.

At the microscopic scale, two models for the interaction between the constituents of a composite are proposed. Finite element models are derived from them, and the results of some calculations that were carried out with these models are presented. The finite element models can be used to calculate the effective properties of the mesodomain.

Keywords

Composites, Micromechanics, Interfaces

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1 Introduction

1.1 Material Models

Material models, or constitutive relations, are essential in describing and analyzing the mechanical behaviour of materials. Theories for developing such models can be divided into two classes: the phenomenological theories and the structural ones. In contrast to the latter, the phenomenological theories do not take into consideration the microstructure of the material. Especially when dealing with composite materials, this microstructure has a significant influence on the mechanical properties of these materials.

The structural theories determine the mechanical properties of a unique fictitious continuous material that 'best' represents the real heterogeneous material or composite. They do take, from the onset, the microstructure of the material into consideration. To that end, they distinguish three different scales. The smallest of these, referred to as the microscopic scale, is the scale of the inhomogeneities, or the constituents of the composite. The second, the mesoscopic scale, is an intermediate scale, which is much larger than the microscale, but still much smaller than the largest, the macroscopic scale. The latter is the scale of the fictitious continuous material.

The structural theories assume that the composite is statistically homogeneous, that is, they assume that all global geometrical characteristics such as volume fractions, etc., are the same in any mesodomain, irrespective of its position. The effective mechanical properties of the mesodomain are obtained from the relations between averages of field variables such as stress and strain. They define the relations between the field variables of the fictitious material. The averages can either be volume averages, or ensemble averages.

The volume average of a field quantity \( f \), over the mesodomain \( M \), is defined by

\[
\bar{f}(x) = \frac{1}{|M|} \int_M f(x,y) \, dy,
\]

where \( x \) is the position vector to a reference point of \( M \), and where \( y \) is the position vector of a material point of \( M \) with respect to \( x \). \( |M| \) is the volume of \( M \). Note that in this case the mesodomain \( M \) is a physical region of the heterogeneous material. Theories based on volume averages can be found in Hill (1965) and Maugin (1992, Chap. 9). While the former deals with linear elastic solids only, the latter also includes elastoplastic (hardening) materials. As shown by Courage (1990), it is also possible to determine the elastic
properties of the mesodomain, by modelling it numerically. In his work, Courage modelled composite materials, reinforced with short fibers, with the finite element method, and calculated the elastic properties of the composites. He assumed perfect bonding between the fibres and the matrix. The disadvantage of this approach is that the calculations may have to be repeated each time another material is considered, since it is virtually impossible to derive closed form expressions for the macroscopic relevant parameters as functions of the structural parameters from the numerical data, especially when the number of structural parameters becomes large.

The ensemble average of the field quantity $f$ is given by

$$\langle f \rangle(x) = \sum_{i=1}^{\infty} p_i f_i(x),$$

where $f_i$ are the possible values of $f$, and where $p_i$ is the probability that $f = f_i$. In this case, the mesodomain $M$ is viewed as a statistical ensemble of microdomains $i = 1, 2, \ldots$, with field quantities $f_i(x)$, and probabilities $p_i$ to 'occur'. Hence, $M$ is a sample space. Theories which are based on ensemble averages are given (amongst others) by Axelrad (1978, 1984), Beran (1968), and Kroner (1971).

If the field variables are statistically homogeneous, that is, if they are statistically indistinguishable within different mesodomains, the volume average and the ensemble average are constant and equal (Hashin 1983).

1.2 Outline of This Report

The main goal of this research project is to derive material models for composite materials, which take into account both the microstructure of the composite and the micromechanical properties of its constituents, as well as their interactions.

We shall present in Chapter 2, for the microscopic level, two micromechanical models for the interaction between the constituents of a composite, in which the stiffness of the interface varies continuously with the displacements of the boundaries of the particles. The models are derived from the one proposed by Axelrad (1978, Sec. 4.2 and 4.3). The latter is based on a finite number of interactions between certain parts of the boundaries of the microparticles. In that chapter, we shall also derive two-, two and a half-, and three-dimensional finite element models, and we shall present the results of some calculations that were carried out with these models.

In the last chapter, some conclusions and subjects for further investigations are discussed.
2 The Interface Between Two Particles

2.1 Introduction

In this chapter we shall present both a continuous and a discrete model for the interaction between two particles. The models are based on the one proposed by Axelrad (1978, Sec. 4.2 and 4.3).

For each particle there will be a part of its surface, the interaction surface, where the particle interacts with the surface of the other particle. In the continuous model, each material point on the interaction surface of a particle interacts with a set of material points on the interaction surface of the other particle. The forces acting between two points are assumed to be conservative with respect to the distance between them, that is, there exists a function $U: [0, \infty) \to \mathbb{R}$, the interaction energy, such that the force that acts on a point $P$ at a distance $r$ of a point $P_0$, due to its interaction with $P_0$, is given by

$$F(r) = -\text{grad} \, U(r) = -F(r) \, e. \quad (2.1)$$

Here, $r$ is the norm of the vector $r$, $e$ is the unit vector in the direction of $r$, and grad is the gradient operator with respect to $r$ (Fig. 2.1). The function $F(r) = U'(r)$ is the magnitude of the force.

In the discrete model, the interaction surfaces of the particles are subdivided into a finite number of subsets, called cells. A cell on the surface of one particle interacts with a family of cells on the surface of the other particle. For the interaction between two cells, a fixed point, the interaction point, is chosen in each of the cells. The (constant) force distribution on a cell, due to the interaction with the other cell, is then given by the force $F(r)$, in which $r$ is the distance vector between the interaction points, multiplied by the area of the other cell.

![Figure 2.1](image.png)

**Figure 2.1** The force $F(r)$ acting on the point $P$ at a distance $r$ of $P_0$, due to its interaction with $P_0$. The vector $e$ is the unit vector in the direction of $r$. 

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Figure 2.2 The potential energy $U(r)$, and the force $F(r) = U'(r)$, of a Lennard-Jones interaction between two molecules, as a function of the separation $r$. The equilibrium separation $r_0$ corresponds to minimal potential energy $-U_0$.

The forces may be due to the molecular attraction between the particles, or they may represent the response of fibrils, formed between them, in cases of crazing, for example. In the former case, if the interface represents the weak Van der Waals interaction between the particles, then the function $U(r)$ is usually taken to be a Lennard-Jones type of potential,

$$U(r) = U_0 \left[ \left( \frac{r_0}{r} \right)^{12} - 2 \left( \frac{r_0}{r} \right)^6 \right], \quad (2.2)$$

where $r_0$ is the equilibrium distance of the bond, corresponding to minimal potential energy $-U_0$. The typical form of both $U(r)$ and $F(r)$ is as depicted in Figure 2.2. Note that $F(r) < 0$ for $r < r_0$, corresponding to repulsion of the two molecules, and that $F(r) > 0$ for $r > r_0$, corresponding to attraction.

In the next section, we shall give the general equations for the two models. In Section 2.3, we shall give a variational formulation of the problem, and we shall present three finite element models for the interaction between the particles: a two-dimensional model, in which the particles are assumed to be in a plane strain or plane stress state, a three dimensional model, and a two and a half-dimensional one, in which the interaction surfaces of the particles are kept parallel. Finally, in Section 2.4, the results of some simple calculations are presented.
2.2 The Equilibrium Equation and The Boundary Conditions

Consider two particles, \( B_1 \) and \( B_2 \), of material points \( P \). Let \( x = \chi(P, t) \) (with \( P \in B_1 \cup B_2 \), and \( t \in T \subseteq \mathbb{R} \)) be the position vector of the material point \( P \) at a time instant \( t \), with respect to the origin of the three-dimensional Euclidean space \( \mathbb{R}^3 \). The region \( \Omega_k = \chi(B_k, t) \), occupied by \( B_k \) at time \( t \), i.e., the set of position vectors of all the material points of the particle, is called the configuration of \( B_k \) at the time \( t \). Let \( \Omega \) be the union of the configurations of \( B_1 \) and \( B_2 \). For convenience, let us choose a reference configuration \( \Omega_r = \Omega_{r,1} \cup \Omega_{r,2} \), for the two particles, and let us identify each material point \( P \) with its position \( X \) in that reference configuration. There now exist a mapping \( \varphi: \Omega_r \times T \rightarrow \Omega \), such that

\[
x = \varphi(X, t).
\]

Let \( \sigma(x, t) \) be the (symmetric) Cauchy stress field on \( \Omega \). If the particles are acted upon by a volume load \( \rho(x, t) b(x, t) \), where \( \rho \) is the mass density of the particles, this field satisfies the local equilibrium equation,

\[
\text{div} \sigma + \rho b = 0, \quad \text{in} \ \Omega \times T,
\]

where \( \text{div} \) is the divergence operator with respect to \( x \).

Let the boundary \( \Gamma_k \) of \( \Omega_k \) be decomposed into three parts: \( \Gamma_k = \Gamma_{u,k} \cup \Gamma_{p,k} \cup \Gamma_{i,k} \). On \( \Gamma_{u,k} \) the positions of the particles are prescribed, while on \( \Gamma_{p,k} \) prescribed boundary loads are acting upon the particles. The part \( \Gamma_{i,k} \) is the interaction surface of the particle. Since the particles are only interacting with each other, there is no resultant force on the interface region, that is, if \( f_k(x, t) \) is the force distribution on \( \Gamma_{i,k} \) (see e.g. (2.11) and (2.12) below), and

\[
F_k(t) = \int_{\Gamma_{i,k}} f_k(x, t) \, d\sigma
\]

is the total force on \( \Gamma_{i,k} \) at time \( t \), we have

\[
F_1(t) + F_2(t) = 0, \quad \text{for all} \ t \in T.
\]

In addition to the local equilibrium equation (2.4), we now have the following set of boundary conditions:

\[
\varphi = \varphi_0(x, t), \quad \text{on} \ \Gamma_u,
\]
\[
t = t_0(x, t), \quad \text{on} \ \Gamma_p,
\]
\[
t = f_k(x, t), \quad \text{on} \ \Gamma_{i,k}, \ \text{for} \ k = 1, 2,
\]

where \( \Gamma_u = \Gamma_{u,1} \cup \Gamma_{u,2} \) and \( \Gamma_p = \Gamma_{p,1} \cup \Gamma_{p,2} \), and where \( t = \sigma n \), with outward normal vector \( n(x, t) \) on \( \Gamma = \Gamma_1 \cup \Gamma_2 \), is the traction vector on the boundaries of the particles. The subscript 0 denotes prescribed quantities. The functions \( f_1 \) and \( f_2 \) have to be chosen such that Equation (2.6) is fulfilled.
2.2.1 The Boundary Loads in the Continuous Model

In the continuous model, we assume that a point \( x_1 \in \Gamma_{i,1} \) interacts with set \( S_2(x_1, t) \) of points \( x_2 \) on \( \Gamma_{i,2} \). Then, obviously, the point \( x_2 \in \Gamma_{i,2} \) interacts with set \( S_1(x_2, t) \subseteq \Gamma_{i,1} \), with

\[
S_1(x_2, t) = \left\{ x_1 \in \Gamma_{i,1} \mid x_2 \in S_2(x_1, t) \right\}
\]  
(2.10)

(\( x_2 \) interacts with all the points \( x_1 \), such that \( x_1 \) interacts with \( x_2 \)). According to (2.1), the force acting on \( x_k \) due to its interaction with \( x_i \) reads \( F(x_k - x_i) \). The total force applied by the set \( S_2(x_1, t) \) to the point \( x_1 \) on \( \Gamma_{i,1} \) is then given by

\[
f_1(x_1, t) = \int_{S_2(x_1, t)} F(x_1 - x_2) \, d\sigma_2, \quad \text{with } x_1 \in \Gamma_{i,1},
\]  
(2.11)

and the total force applied by the set \( S_1(x_2, t) \) to \( x_2 \in \Gamma_{i,2} \) reads

\[
f_2(x_2, t) = \int_{S_1(x_2, t)} F(x_2 - x_1) \, d\sigma_1, \quad \text{with } x_2 \in \Gamma_{i,2}.
\]  
(2.12)

The latter equations give us the desired boundary loads on the interaction surfaces of the particles. To show that they satisfy (2.6), note that

\[
F(-r) = -F(r), \quad \text{and because } x_1 \text{ is an element of } S_1(x_2, t) \text{ if and only if } x_2 \text{ is an element of } S_2(x_1, t) \text{ (cf. (2.10))}, \text{ it follows that the sum } F_1 + F_2 \text{ indeed vanishes.}
\]

2.2.2 The Boundary Loads in the Discrete Model

In the discrete model, we choose a subdivision \( \{ C_{kn} \subseteq \Gamma_{i,k} \mid n = 1, 2, \ldots, N_k \} \), with \( N_k \in \mathbb{N} \), of cells on \( \Gamma_{i,k} \), such that

\[
\bigcup_{n=1}^{N_k} C_{kn} = \Gamma_{i,k} \quad \text{and} \quad C_{kn} \cap C_{km} = \emptyset, \quad \text{if } n \neq m.
\]  
(2.15)

We assume that the cell \( C_{1n_1} \) of \( B_1 \) interacts with the family \( \{ C_{2n_2} \mid n_2 \in I_{2n_1} \} \) of cells of \( B_2 \), where \( I_{2n_1} \) is some subset of \( \{1, 2, \ldots, N_2\} \). Then \( C_{2n_2} \) interacts with the family \( \{ C_{1n_1} \mid n_1 \in I_{1n_2} \} \), where \( I_{1n_2} \) is given by

\[
I_{1n_2} = \left\{ n_1 \in \{1, 2, \ldots, N_1\} \mid n_2 \in I_{2n_1} \right\}
\]  
(2.16)
Finite Element Models for the Interface

Let $\xi_{kn} \in C_{kn}$ be the interaction point of the cell $C_{kn}$. The force acting on the points $x$ in the cell $C_{kn}$, due to the interaction of this cell with $C_{lm}$ is given by $F(\xi_{kn} - \xi_{lm}) \mu(C_{lm})$, where $\mu(A) = \int_A d\sigma$ is the area of the set $A$. The load distributions $f_1(x,t)$ on $\Gamma_{i,k}$ are now readily seen to be

\[ f_1(x_1, t) = \sum_{n_2 \in I_{2n_2}} F(\xi_{1n_1} - \xi_{2n_2}) \mu(C_{2n_2}), \quad \text{if} \ x_1 \in C_{1n_1}, \tag{2.17} \]

\[ f_2(x_2, t) = \sum_{n_1 \in I_{1n_1}} F(\xi_{2n_2} - \xi_{1n_1}) \mu(C_{1n_1}), \quad \text{if} \ x_2 \in C_{2n_2}. \tag{2.18} \]

Note that the total forces $F_1$ and $F_2$ on $\Gamma_{i,1}$ and $\Gamma_{i,2}$, respectively, are given by

\[ F_1(t) = \int_{\Gamma_{i,1}} f_1(x, t) d\sigma = \sum_{n_1 = 1}^{N_1} \mu(C_{1n_1}) \sum_{n_2 \in I_{2n_2}} F(\xi_{1n_1} - \xi_{2n_2}) \mu(C_{2n_2}), \tag{2.19} \]

\[ F_2(t) = \int_{\Gamma_{i,2}} f_2(x, t) d\sigma = \sum_{n_2 = 1}^{N_2} \mu(C_{2n_2}) \sum_{n_1 \in I_{1n_1}} F(\xi_{2n_2} - \xi_{1n_1}) \mu(C_{1n_1}), \tag{2.20} \]

and that since $n_2 \in I_{2n_1}$ if and only if $n_1 \in I_{1n_2}$ (cf. (2.16)), the sum of these forces vanishes, hence these load distributions satisfy (2.6) too.

Notice further that if a cell $C_{kn}$ interacts with all the cells $C_{lm}$ within a fixed part of the interaction surface of $B_i$, and if the subdivision of cells on $\Gamma_{i,l}$ is getting finer and finer, i.e., if $\mu(C_{lm}) \to 0$, the sums in (2.17) and (2.18) converge (if they converge) to the integrals in (2.11) and (2.12). The continuous model can thus be seen as a limit case of the discrete model.

### 2.3 Finite Element Models for the Interface

We shall now give a variational formulation of the problem formed by the Eqns. (2.4)–(2.9), where the functions $f_1(x,t)$ and $f_2(x,t)$ are given either by (2.11) and (2.12), or by (2.17) and (2.18) (see also Johnson (1987, Sec. 5.1)).

Let $v(x)$ be a test function on $\Omega$ such that $v = 0$ on $\Gamma_u$. Scalar multiplication of the local equilibrium equation (2.4) with $v$, and integration over $\Omega$, yields

\[ \int_\Omega (\text{div} \sigma + \rho b, v) \, dx = 0. \tag{2.21} \]

Since $\text{div}(\sigma v) = (\text{div} \sigma, v) + \text{tr} [\sigma \text{grad} v]$, it follows that

\[ \int_\Omega (\text{div} \sigma, v) \, dx = \int_\Omega (t, v) \, d\sigma - \int_\Omega \text{tr} [\sigma \text{grad} v] \, dx, \tag{2.22} \]

where we have also used Gauss’ Divergence Theorem, the symmetry of $\sigma$, and the definition of the traction vector. With this relation, the boundary conditions (2.8) and (2.9), and
with the fact that \( v = 0 \) on \( \Gamma_u \), Equation (2.21) leads us to the following variational problem: find \( \varphi \) such that \( \varphi = \varphi_0 \) on \( \Gamma_u \), and such that

\[
\int_\Omega \text{tr}[\mathbf{\sigma}(\text{grad } v)] \, dx - \int_{\Gamma_{1,1}} (f_1, v) \, d\sigma - \int_{\Gamma_{1,2}} (f_2, v) \, d\sigma = \int_\Omega (\rho \, b, v) \, dx + \int_{\Gamma_p} (t_0, v) \, d\sigma, \tag{2.23}
\]

for every \( v(x) \) that vanishes on \( \Gamma_u \).

### 2.3.1 A Two-dimensional Finite Element Model for the Interface

Let us assume that the particles \( B_1 \) and \( B_2 \) are in a plane strain or plane stress state. In that case, the problem (2.4)–(2.9) reduces to a two-dimensional problem, in which the configurations are now bounded regions in \( \mathbb{R}^2 \) and their boundaries are simple closed arcs.

Let us choose, for the finite element model, a triangulation of the particles, such that these arcs are interpolated piecewise linearly (e.g., by using four-noded quadrilateral elements, or three-noded triangular elements). Let \( P_{k1} \) and \( P_{k2} \) be two consecutive nodes on \( \Gamma_{i,k} \), and let \( x_{k1} \) and \( x_{k2} \) be their respective positions at time \( t \) (Fig. 2.3). Let \( \Lambda_k \subset \Gamma_{i,k} \) be the line segment between them, given by the parametric representation

\[
\varphi|_{\Lambda_k} = \varphi_k(u) = \sum_{i=1}^{2} \psi_i(u) x_{ki}, \quad \text{for } u \in [0,1), \tag{2.24}
\]
Finite Element Models for the Interface

in which \( \psi_1(u) = 1 - u \), and \( \psi_2(u) = u \). We shall use a Galerkin method, that is, we shall interpolate the test functions \( v(x) \) on \( \Lambda_k \) accordingly:

\[
v|_{\Lambda_k} = \sum_{i=1}^{2} \psi_i(u) v_{ki}, \quad \text{for } u \in [0,1),
\]

(2.25)

with \( v_{ki} = v(x_{ki}) \). With these relations, the contribution to the variational formulation (2.23) of the interaction between the boundaries \( \Lambda_1 \) and \( \Lambda_2 \) (i.e., the second and third term on the left hand side of (2.23)) can be written as

\[
\int_{\Lambda_1} (f_1,v) d\sigma + \int_{\Lambda_2} (f_2,v) d\sigma = \sum_{k=1}^{2} \sum_{i=1}^{2} (K_{ki},v_{ki}),
\]

(2.26)

where \( K_{ki} \) are the generalized forces at the nodes \( P_{ki} \), given by

\[
K_{ki} = \int_0^1 \psi_i(u) f_k(\varphi_k(u), t) \| \dot{\varphi}_k(u) \| du.
\]

(2.27)

Note that \( \| \dot{\varphi}_k(u) \| = \| x_{ki} \| = \ell_k \) is the length of \( \Lambda_k \).

The Generalized Forces in the Continuous Model

For the continuous model, we assume that a point \( u \in [0,1) \) interacts with the points \( v \) of the set

\[
S(u) = \{ v \in [0,1) \mid |v - u| \leq a \},
\]

(2.28)

in which \( a > 0 \). By (2.24), we have for a point \( x_1 = \varphi_1(u_1) \in \Lambda_1 \), and a point \( x_2 = \varphi_2(u_2) \in \Lambda_2 \),

\[
x_2 - x_1 = \sum_{i=1}^{2} [\psi_i(u_2)x_{2i} - \psi_i(u_1)x_{1i}] =: r(u_2, u_1),
\]

(2.29)

so that, according to (2.11) and (2.12), the load distributions \( f_k(\varphi_k(u), t) \) on \( \Lambda_k \) read

\[
f_1(\varphi_1(u_1), t) = -\int_{S(u_1)} F(r(u_2, u_1)) \| \dot{\varphi}_2(u_2) \| du_2,
\]

(2.30)

\[
f_2(\varphi_2(u_2), t) = \int_{S(u_2)} F(r(u_2, u_1)) \| \dot{\varphi}_1(u_1) \| du_1.
\]

(2.31)

Here, we have used the fact that \( F(-r) = -F(r) \). Substituting these relations into (2.27), finally yields the generalized forces at the nodes in the continuous model,

\[
K_{1i} = -\int_0^1 \psi_i(u_1) \| \dot{\varphi}_1(u_1) \| du_1 \int_{S(u_1)} F(r(u_2, u_1)) \| \dot{\varphi}_2(u_2) \| du_2,
\]

(2.32)

\[
K_{2i} = \int_0^1 \psi_i(u_2) \| \dot{\varphi}_2(u_2) \| du_2 \int_{S(u_2)} F(r(u_2, u_1)) \| \dot{\varphi}_1(u_1) \| du_1.
\]

(2.33)
The Generalized Forces in the Discrete Model

For the discrete model, we choose a uniform subdivision of cells $C_{kn}$ on $\Lambda_k$, according to

$$C_{kn} = \{ x = \varphi_k(u) \mid (n-1)h \leq u < nh \}, \quad \text{for } n = 1, 2, \ldots, N,$$

(2.34)

with $N \in \mathbb{N}$ and $h = 1/N$, and we choose the center $x_{kn} = \varphi_k(\nu_n)$, with $\nu_n = (n - \frac{1}{2})h$, of the cell $C_{kn}$ to be its interaction point. Suppose that the cell $C_{kn}$ interacts with the cells $C_{im}$, for $m \in I_n$, with

$$I_n = \{ m \in \{1, 2, \ldots, N\} \mid |m - n| \leq b \},$$

(2.35)

where $b > 0$. In this case, the load distributions $f_k(\varphi(u), t)$ are given by (2.17) and (2.18), yielding

$$f_1(\varphi_1(u), t) = -A_2 \sum_{n_2 \in I_{n_1}} F(r(\nu_{n_2}, \nu_{n_1})), \quad \text{for } u \in [(n_1 - 1)h, n_1h),$$

(2.36)

$$f_2(\varphi_2(u), t) = A_1 \sum_{n_1 \in I_{n_2}} F(r(\nu_{n_2}, \nu_{n_1})), \quad \text{for } u \in [(n_2 - 1)h, n_2h),$$

(2.37)

in which $A_k = \mu(C_{kn}) = h\ell_k$ is the 'area' of $C_{kn}$. Substituting these relations into (2.27) we obtain the generalized forces at the nodes, for the discrete model,

$$K_{1i} = -h^2\ell_1\ell_2 \sum_{n_1=1}^{N} \alpha_{in_1} \sum_{n_2 \in I_{n_1}} F(r(\nu_{n_2}, \nu_{n_1})), \quad \text{(2.38)}$$

$$K_{2i} = h^2\ell_1\ell_2 \sum_{n_2=1}^{N} \alpha_{in_2} \sum_{n_1 \in I_{n_2}} F(r(\nu_{n_2}, \nu_{n_1})), \quad \text{(2.39)}$$

in which

$$\alpha_{in} = \frac{1}{h} \int_{(n-1)h}^{nh} \psi_i(u) \, du = \begin{cases} 1 - (n - \frac{1}{2})h, & \text{if } i = 1, \\ (n - \frac{1}{2})h, & \text{if } i = 2. \end{cases} \quad \text{(2.40)}$$

The Derivatives of the Generalized Forces

Since, in general, the variational problem (2.23) is a nonlinear relation for $\varphi$, it must be solved numerically, for example using a Newton-Raphson iterative procedure. For such a procedure we need to linearize the equation. In particular, we need the derivatives of the generalized forces $K_{ki}$ with respect to the position vectors $x_{ij}$. We see from Equations (2.27), (2.32) and (2.33), and (2.38) and (2.39), that calculating these derivatives amounts to determining the derivative $\mathcal{K}_{ij} = \partial k/\partial x_{ij}$, with $k$ given by

$$k(x_{11}, x_{12}, x_{21}, x_{22}; u_1, u_2) = \| \dot{\varphi}_1(u_1) \| \| \dot{\varphi}_2(u_2) \| F(r(u_2, u_1)).$$

(2.41)
By (2.24), we have
\[
\frac{\partial \| \phi_k(u) \|}{\partial x_{ij}} = \delta_{kl} \psi_j(u) \frac{\phi_k(u)}{\| \phi_k(u) \|},
\] (2.42)
in which \( \delta_{kl} \) is Kronecker's delta. Using (2.29), we see that we can write \( K_{1j} \) and \( K_{2j} \) as
\[
K_{1j} = \psi_j(u_1) \| \phi_2(u_2) \| \mathbf{F}(\mathbf{r}(u_2, u_1)) \otimes \frac{\phi_1(u_1)}{\| \phi_1(u_1) \|}
- \psi_j(u_1) \| \phi_1(u_1) \| \| \phi_2(u_2) \| \mathbf{F},
\] (2.43)
\[
K_{2j} = \psi_j(u_2) \| \phi_1(u_1) \| \mathbf{F}(\mathbf{r}(u_2, u_1)) \otimes \frac{\phi_2(u_2)}{\| \phi_2(u_2) \|}
+ \psi_j(u_2) \| \phi_1(u_1) \| \| \phi_2(u_2) \| \mathbf{F},
\] (2.44)
in which \( a \otimes b \) is the tensor product of the vectors \( a \) and \( b \), and where \( \mathbf{F} \) is the derivative \( \partial \mathbf{F}/\partial \mathbf{r} \) in \( \mathbf{r}(u_2, u_1) \). The latter can be obtained from (2.1), yielding
\[
\frac{\partial \mathbf{F}(\mathbf{r})}{\partial \mathbf{r}} = - \left[ \mathbf{F}'(\mathbf{r}) - \frac{\mathbf{F}(\mathbf{r})}{\mathbf{r}} \right] \mathcal{E}(\mathbf{r}) - \frac{\mathbf{F}(\mathbf{r})}{\mathbf{r}} \mathcal{I}
\] (2.45)
where \( \mathcal{E}(\mathbf{r}) \) is the projection operator on \( \mathbf{e} = \mathbf{r}/\| \mathbf{r} \| \), defined by
\[
\mathcal{E}(\mathbf{r}) \mathbf{x} = (\mathbf{e}, \mathbf{x}) \mathbf{e} \quad (\mathbf{x} \in \mathbb{R}^2),
\] (2.46)
and \( \mathcal{I} \) is the identity operator.

### 2.3.2 A Three-dimensional Finite Element Model for the Interface

Since we need the results in the next subsection, we shall now briefly discuss a three-dimensional finite element model.

Let us choose a triangulation for the particles (e.g., consisting of eight-noded brick elements) such that the part \( E_k \) of the boundary \( \Gamma_{i,k} \) within one element is a quadrilateral with nodes \( P_{ki} \) at its vertices. Suppose that it is interpolated bilinearly, that is, it can be given by the parametric representation
\[
\varphi|_{E_k} = \varphi_k(u, v) = \sum_{i=1}^4 \psi_i(u, v) x_{ki}, \quad \text{with } (u, v) \in [0,1) \times [0,1),
\] (2.47)
where \( x_{ki} \) are the position vectors, at time \( t \), of the nodes \( P_{ki} \), of the element at the boundary, and where \( \psi_1(u, v) = (1 - u)(1 - v), \psi_2(u, v) = u(1 - v), \psi_3(u, v) = uv, \) and \( \psi_4(u, v) = (1 - u)v \). Again, we shall interpolate the test functions \( \mathbf{v}(\mathbf{x}) \) on \( E_k \) accordingly:
\[
\mathbf{v}|_{E_k} = \sum_{i=1}^4 \psi_i(u, v) \mathbf{v}_{ki}, \quad \text{for } (u, v) \in [0,1) \times [0,1),
\] (2.48)
with $v_{ki} = v(x_{ki})$. If we substitute these relations into the variational problem (2.23), we obtain for the contribution of the interface between the parts $E_1$ and $E_2$ to that relation an equation similar to (2.26):

$$
\int_{E_1} (f_1, v) \, d\sigma + \int_{E_2} (f_2, v) \, d\sigma = \sum_{k=1}^{4} \sum_{i=1}^{4} (K_{ki}, v_{ki}),
$$

(2.49)

where the generalized forces $K_{ki}$ at the nodes $P_{ki}$, are now given by

$$
K_{ki} = \int_0^1 du \int_0^1 \psi_i(u,v) f_i(\varphi_i(u,v),t) \left( \frac{\partial \varphi_k}{\partial u} \times \frac{\partial \varphi_k}{\partial v} \right) \, dv.
$$

(2.50)

The Generalized Forces in the Continuous Model

For the continuous model we assume that a point $(u,v) \in [0,1] \times [0,1)$ interacts with the points $(w,z) \in S(u) \times S(v)$, where $S$ is given by (2.28). The load distributions on $E_1$ and $E_2$ are then again obtained from (2.11) and (2.12). With $r(u_2,v_2;u_1,v_1)$ set to

$$
r(u_2,v_2;u_1,v_1) = \varphi_2(u_2,v_2) - \varphi_1(u_1,v_1) = \sum_{i=1}^{4} \left[ \psi_i(u_2,v_2) x_{2i} - \psi_i(u_1,v_1) x_{1i} \right],
$$

(2.51)

they become

$$
f_1(\varphi_1(u_1,v_1),t) = - \int_{S(u_1)} du_2 \int_{S(v_1)} F(r(u_2,v_2;u_1,v_1)) \left( \frac{\partial \varphi_2}{\partial u_2} \times \frac{\partial \varphi_2}{\partial v_2} \right) \, dv_2,
$$

(2.52)

$$
f_2(\varphi_2(u_2,v_2),t) = \int_{S(u_2)} du_1 \int_{S(v_2)} F(r(u_2,v_2;u_1,v_1)) \left( \frac{\partial \varphi_1}{\partial u_1} \times \frac{\partial \varphi_1}{\partial v_1} \right) \, dv_1.
$$

(2.53)

Substitution of these relations into (2.50), yields the generalized forces at the nodes.

The Generalized Forces in the Discrete Model

For the discrete model, we choose again a uniform subdivision of cells $C_{kmn}$ on $E_k$, according to

$$
C_{kmn} = \left\{ x = \varphi_k(u,v) \mid (m-1)h < u < mh, \ (n-1)h < v < nh \right\},
$$

(2.54)

for $m, n = 1, 2, \ldots, N$, and we choose the center $\xi_{kmn} = \varphi_k(\nu_m, \nu_n)$ to be the interaction point of $C_{kmn}$. Further, we assume that the cell $C_{kmn}$ interacts with the cells $C_{pq}$, for $(p, q) \in I_m \times I_n$, with $I_n$ given by (2.35). The load distributions on $E_1$ and $E_2$ then read

$$
f_1(\varphi_1(u_1,v_1),t) = - \sum_{m_2 \in I_{m_2}} \sum_{n_2 \in I_{n_2}} F(\varphi_{m_2}, \nu_{n_2}; \nu_{m_1}, \nu_{n_1}) A_{2m_2n_2},
$$

(2.55)

$$
f_2(\varphi_2(u_2,v_2),t) = \sum_{m_1 \in I_{m_1}} \sum_{n_1 \in I_{n_1}} F(\varphi_{m_2}, \nu_{n_2}; \nu_{m_1}, \nu_{n_1}) A_{1m_1n_1},
$$

(2.56)
where
\[
A_{k_mn} = \int_{(m-1)h}^{mh} du \int_{(n-1)h}^{nh} \left( \frac{\partial \varphi_k}{\partial v} \times \frac{\partial \varphi_k}{\partial u} \right) dv
\]  
(2.57)

is the area of the cell \( C_{k_mn} \). Substitution of these relations into (2.50), yields the generalized forces at the nodes.

The derivatives \( \partial K_{ki}/\partial x_{ij} \) can be calculated using the same procedure as in the preceding subsection.

### 2.3.3 A Two And A Half-dimensional Finite Element Model of the Interface

Since from a numerical point of view a two-dimensional model is preferable to a three-dimensional one (less degrees of freedom), we shall derive from the three-dimensional model presented in the preceding subsection, a two and a half-dimensional model, by demanding that the nodes \( P_{ki} \), for \( i = 1, 2, 3 \) and \( 4 \), all stay in one fixed plane, and by requiring that the two planes (for \( k = 1, 2 \)) are parallel, at a distance \( d \) of each other. Let \( n \) be the (unit) normal to both the planes. Without loss of generality, we can set
\[
x_{1i} = \bar{x}_{1i} - \frac{1}{2} d n \quad \text{and} \quad x_{2i} = \bar{x}_{2i} + \frac{1}{2} d n, \tag{2.58}
\]
where \( \bar{x}_{ki} \) is the component of \( x_{ki} \) perpendicular to \( n \), i.e., \( (\bar{x}_{ki}, n) = 0 \). The parametric representations \( \varphi_1(s, t) \) and \( \varphi_2(s, t) \) of \( E_1 \) and \( E_2 \) can then also be split into their components parallel and normal to \( n \):
\[
\varphi_1(u, v) = \bar{\varphi}_1(u, v) - \frac{1}{2} d n \quad \text{and} \quad \varphi_2(u, v) = \bar{\varphi}_2(u, v) + \frac{1}{2} d n, \tag{2.59}
\]
with
\[
\bar{\varphi}_k(u, v) = \sum_{i=1}^{4} \psi_i(u, v) \bar{x}_{ki}. \tag{2.60}
\]

The distance vector \( r = x_2 - x_1 \) between a point \( x_2 \in E_2 \), and a point \( x_1 \in E_1 \), can now be written as \( r = \bar{r} + d n \), where \( \bar{r} \) is perpendicular to \( n \). By (2.1) we obtain for the force \( F(\bar{r} + d n) \),
\[
F(\bar{r} + d n) = -F\left( \sqrt{\bar{r}^2 + d^2} \right) \frac{\bar{r} + d n}{\sqrt{\bar{r}^2 + d^2}} = \bar{F}(\bar{r}) d + F^\perp(\bar{r}, d) n, \tag{2.61}
\]
with \( \bar{r} = ||\bar{r}|| \), and
\[
\bar{F}(\bar{r}, d) = -F\left( \sqrt{\bar{r}^2 + d^2} \right) \frac{\bar{F}}{\sqrt{\bar{r}^2 + d^2}}, \tag{2.62}
\]
\[
F^\perp(\bar{r}, d) = -F\left( \sqrt{\bar{r}^2 + d^2} \right) d \frac{\bar{F}}{\sqrt{\bar{r}^2 + d^2}}. \tag{2.63}
\]
If we substitute these relations into (2.52) and (2.53), or into (2.55) and (2.56), and use the resulting relations in (2.50), we obtain the generalized forces $K_{ki}$ at the nodes. These forces can also be split into their components $K^+_{ki}$ in the direction of $n$, and $K^-_{ki}$ perpendicular to $n$. They are functions of the positions $x_{ij}$ of the nodes, and of the thickness $d$ of the interface. There are two ways to arrive at a two-dimensional model:

(i) Keep the thickness $d$ of the interface fixed and neglect the forces normal to the planes (i.e., $K_{ki}^-$. The forces $K_{ki}^+$ are taken as functions of the positions $x_{ij}$ of the nodes in the plane. The derivatives of the forces can be calculated with the same procedure as in Section 2.3.1. In this case, however, there will be a non-zero resultant force

$$K_k^+ = \sum_{i=1}^{4} K_{ki}^+$$  \hspace{1cm} (2.64)

perpendicular to $E_k$.

(ii) Choose the thickness $d$ such that the forces $K_{ki}^+$ vanish. This, however, gives an additional equation to the resulting set of equations for the positions of the nodes.

In the next section we shall see that if we choose for the first option, the calculated forces $K_k^+$, can become very large (much larger than the forces in the plane).

2.4 Results of Some Simple Calculations

In this section, we shall give the results of some simple calculations, based on the two- and two and a half-dimensional models, presented in the preceding section.

In all the calculations the particles were homogeneous isotropic elastic bodies, and all triangulations were made up by bilinear quadrilateral elements. Further, only the discrete variants of the models were used, in which a cell $C_{kn}$ interacts with the cells $C_{l,n-b}$, $C_{l,n-b+1}$, ..., $C_{l,n}$, ..., $C_{l,n+b-1}$, and $C_{l,n+b}$. In most of the tests $b$ was chosen equal to 1, but in the pullout test $b$ was set to 1, 2, 5, and 10, respectively. For the interaction energy between two points, the Lennard-Jones potential (2.2) was taken.

2.4.1 Calculations With the Two-dimensional Model

As a first example of the two-dimensional interface model, a peel-off test was simulated. In this test, a thin elastic plate with cross-section $CDFE$ is glued to a rigid surface $AB$ (Fig. 2.4). The side $DF$ of the plate is clamped, while the displacement $u$ of the point $E$ is prescribed in the vertical direction (i.e., normal to the plate). The sides $CD$ and $AB$ are the 'surfaces' where the interaction between the plate and the rigid surface is taken place. The vertical component of the force $F$, acting on $E$, is plotted in Figure 2.5, as a function of $u$. The straight line in that plot shows the force in case the interaction between the
Results of Some Simple Calculations

Figure 2.4 The cross-section $CDFE$ of an elastic plate glued to the rigid surface $AB$, for a peeloff test. The side $DF$ is clamped, while the displacement $u$ of the point $E$ is prescribed in the direction normal to the plane. The sides $CD$ and $AB$ are the interaction surfaces of the plate and the rigid surface, respectively.

Figure 2.5 The vertical component of the force $F$ applied to the point $E$ as a function of the vertical component of the displacement $u$ of that point. The straight line shows the force in case the interaction between the plate and the surface is omitted.
plate and the surface is omitted. We see that the force in the peel-off test converges to this one. It is caused by the fact that the Lennard-Jones force decreases rapidly to zero, after having reached its maximum at $r = r_0$ (Fig. 2.2). Hence, if the displacement of the point $C$ normal to $AB$ is large enough, the interaction between the two surfaces vanishes.

The second example of the two-dimensional interface model is the fibre pullout test. In this test, a fibre, initially embedded in a matrix, is being pulled out. The initial configuration is depicted in Figure 2.6. Because of the symmetry of the problem only half of the composite is modelled. The sides $HGE$ are clamped, while the displacements in the vertical direction of $AB$ are suppressed. The sides $CD$ and $EF$ are the interaction surfaces of the matrix and the fibre. The horizontal component of the force $F$ applied to the fibre end $BD$ is plotted in Figure 2.7 as a function of its horizontal displacement, for different values of $b$. We observe that for higher values of $b$, the interface 'collapses' at larger displacements of the fibre end. This is because the 'area' of the cells is equal in all four cases, and hence the total 'area' with which a cell interacts increases if $b$ increases.

Note that the interface doesn't collapse in the real sense of the word, since the model used here is a purely elastic one: if the load would be removed from the fibre end, both the fibre and the matrix would return to their initial configuration.

2.4.2 Calculations With the Two And A Half-dimensional Model

In order to test the two and a half-dimensional model, two squares $ABCD$ and $EFGH$ (Fig. 2.8) of the same size where placed parallel to each other at a fixed distance (i.e., we used the first option of Section 2.3.3). The point $A$ was fixed, and the displacement of point $B$ in the $y$-direction was suppressed. The points $E$, $F$, $G$, and $H$ of the upper square where rotated about the center of the square. In Figure 2.9 the forces $K_{21,x}$ and $K_{21,y}$ at the point $E$, and the resultant force $F_z$ on the upper square are plotted as functions of the rotation angle $\varphi$. From this figure we see what we indicated in Section 2.3.3, namely that the resultant force normal to the squares is much larger than the forces in the plane.

In the final example, a three by three square network of overlapping fibres was modelled under a diagonal loading (Fig. 2.10a). In the squares marked with a circle ($\circ$), two fibres overlap. At those points two quadrilateral elements are placed on top of each other, as in Figure 2.9. These elements are kept at a fixed distance from each other, in the direction normal to the plane. They interact according to the two and a half-dimensional model. The point $A$ is fixed, while the displacements of the point $B$ are prescribed along the diagonal through $A$ and $B$. In Figure 2.10 three deformed configurations of the network are depicted. The third one is very near the point where the network 'collapses', that is, where the interfaces between the fibres 'break'. Again, the interface doesn't really break. Finally, the force in the horizontal direction at the point $B$ is plotted in Figure 2.11, as a function of the displacement of that point in that direction.
Figure 2.6 The initial configuration of the fibre $ABDC$ in the matrix $EFHG$. The region $CDFE$ is the interface between matrix and fibre.

Figure 2.7 The horizontal component of the force $F$ applied to the fibre end $BD$ as a function of its horizontal displacement $u_x$, for different values of $b$. 
Figure 2.8 Two interacting parallel squares $ABCD$ and $EFGH$ at a fixed distance of each other.

Figure 2.9 The forces $\bar{K}_{21,x}$ and $\bar{K}_{21,y}$ exerted on the point $E$ in the plane and the resultant force $K_2^\perp$ on the upper square as a function of the rotation angle $\varphi$. 
Figure 2.10 The initial configuration (a) and three deformed states of a three by three square network of overlapping fibres. In the squares marked with a circle (c), two quadrilateral elements are placed on top of each other (Fig. 2.9). The point A is fixed (that is, both the nodes in that point), while the point B is displaced along the diagonal through A and B. The deformed configurations are taken at displacements $u = (1, 1)$ (b), $u = (2, 2)$ (c) and $u = (3, 3)$ (d).
Figure 2.11 The force $F_z$ in the horizontal direction applied to the point $B$ as a function of the displacement $u_z$ of that point in the same direction.
3 Conclusions and Further Investigations

In Chapter 2, we presented two models for the interaction between two particles. In addition, we derived finite element models from them, for two-, two and a half-, and three-dimensional finite element calculations. The models can be used in a wide range of applications. For example, for the fibre-matrix interface, as in the second example of Section 2.4, or fibre-fibre interface in a (two-dimensional) fibre network, as in the fourth example of that section.

The finite element models are purely elastic since each point on the interaction surface of a particle interacts with a fixed part of the interaction surface of the other particle, and the interaction between two points is elastic. However, they can be extended without much effort to, for example, elastoplastic (hardening and softening) models.

In order to determine the effective material properties of the mesodomain, we need to derive the relation between averages (either volume or ensemble averages) of stress and strain in the mesodomain. For this, we can use one of the theories discussed in Chapter 1. However, all these theories deal with linear elastic solids (except Maugin (1992, Chap. 9), who also includes elastoplastic materials), while we have seen in Chapter 2, that the interface behaves nonlinearly. We thus have to investigate whether—and if so, how—these theories can be extended to nonlinear problems.

With the finite element models, we can use Courage's method (Courage 1990)—which can be extended relatively easy to nonlinear problems—to calculate the mesoscopic properties. However, as we already stated in the introduction to this report, it is virtually impossible to derive closed form expressions for these properties as functions of the microscopic ones from the numerical data.
References


