Multiscale failure modelling of quasi-brittle materials
Multiscale failure modelling of quasi-brittle materials

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Summary

Multiscale failure modelling of quasi-brittle materials
by V.P. Nguyen

The conventional multiscale homogenization theory, which has mainly been applied to determine constitutive laws for bulk materials, suffers from two drawbacks when applied to softening materials. Firstly, the coarse scale response is sensitive to the finite element mesh used to discretize the coarse scale domain. Secondly, increasing the size of the fine scale model does not lead to a converged homogenized response. In other words, a Representative Volume Element (RVE) does not exist for softening materials in the classical sense of homogenization.

This work aims at devising a computational homogenization (CH) method, which is objective with respect to the (finite element) discretizations of the coarse scale/fine scale models and to the fine scale model size (size of a material sample upon which a fine scale model is applied). The method is applied to softening quasi-brittle materials. These materials have a random heterogeneous microstructure that undergoes localized damage such as concrete.

The concept of an RVE for quasi-brittle softening materials has been revisited in this work in which we developed a new averaging technique coined the *failure zone averaging scheme*. The basic idea of the scheme is to do the averaging over a propagating damaged zone, rather than over the entire fine scale domain. By doing so, we have been able to obtain homogenized initially rigid cohesive laws which are independent of fine scale model size (when this size is larger than a minimum value in order for the fine scale model to be independent of the microstructural randomness) which allows us to state that an RVE exists for softening materials when averaging towards a coarse scale cohesive law.

Two CH based multiscale cohesive crack frameworks are developed by which the two aforementioned drawbacks associated with conventional homogenization theories applied for softening materials are eliminated. Ac-
cording to the first framework, referred to as a discontinuous homogeniza-
tion scheme, the coarse scale bulk material is assumed to be linear elastic
with effective properties computed a priori while the behavior of the coarse
scale cohesive crack is coming from nested finite element computations per-
formed on a fine scale model (in the spirit of FE² methods). The method pro-
vides an energetically equivalent means to upscale a fine scale localization
band to a coarse scale cohesive crack. Due to the assumption on the elas-
tic behaviour of the coarse scale bulk, the number of nested finite element
models is limited e.g., equals the number of integration points locating on
the coarse scale cracks thus reducing the computational expense. The sec-
ond computational homogenization procedure that has been developed in
this thesis is referred to as a continuous-discontinuous CH scheme. Accord-
ing to the second CH scheme, constitutive behaviour of the bulk material
as well as that of the cohesive crack at the coarse scale are determined from
nested fine scale finite element computations. Although computationally ex-
pensive, the continuous-discontinuous homogenization scheme is more ac-
curate than the discontinuous CH scheme for problems in which the energy
dissipated prior to fine scale localization is significant. The models are ver-
ified against direct numerical simulations (DNS) and numerical examples
show that with CH models, significantly reduced computational expense
has been obtained compared to DNS without compromising the accuracy.

Also presented in this thesis is a multiscale framework for modelling het-
erogeneous material layers. At the coarse scale, they are modelled by zero-
thickness interface elements of which an initially elastic cohesive law is de-
derived from a fine scale model. A new solution scheme to solve the coupled
system of equations (the fine scale equilibrium equation and the fine/coarse
scale transition equation) is presented.

A fully numerical framework to study the mechanical behavior of harden-
ing cement pastes is developed in this dissertation. Based on this microme-
chanical model, a macro-meso-micro three scale model for concrete is pro-
posed. In order to make multiscale simulations feasible, parallelization of
the multiscale code is realized by solving the fine scale models in parallel.
Samenvatting

Een multische aanpak voor het modelleren van schade aan semi-brosse materialen
door V.P. Nguyen

De klassieke aanpak voor het homogeniseren van materiaaleigenschappen, die hoofdzakelijk wordt toegepast ter bepaling van de effectieve eigenschappen van bulk materialen, kent twee belangrijke nadeelen wanneer ze wordt gebruikt voor softening materialen. Ten eerste is het macrogedrag van het materiaal gevoelig voor de fijnheid waarmee dat domein wordt discretiseerd. Ten tweede convergeert het gehomogeniseerde gedrag niet bij een toenemende afmeting van het onderliggende micromodel. Met andere woorden, bij een klassieke homogenisatieaanpak blijkt een Representatief Volume Element (RVE) dus niet te bestaan.

In dit proefschrift wordt een Numerieke Homogenisatiemethode (NH) geïntroduceerd die bovenstaande nadelen ondervangt. De methode wordt toegepast op semi-brosse materialen die softening gedrag vertonen. Deze materialen hebben een willekeurige heterogene microstructuur waarbij optredende schade sterk lokaliseert zoals in beton. Een nieuwe middelingmethode genaamd “failure zone averaging scheme” wordt gebruikt ter bepaling van de RVE voor semi-brosse softening materialen. Het idee achter deze methode is om alleen te middenen over het beschadigde gebied van het micromodel in plaats van over het gehele domein. Op deze manier zijn we in staat om gehomogeniseerde cohesie-eigenschappen van het materiaal te verkrijgen die, vanaf een bepaalde minimumaafmeting (zodat de microstructuur statistisch gezien willekeurig is), onafhankelijk worden van de afmetingen van het micromodel. Dit toont het bestaan aan van een RVE voor de bepaling van effectieve cohesie-eigenschappen van dergelijke materialen.

Twee op de NH gebaseerde raamwerken voor de multischaalsimulaties van cohesieve scheurvorming in softening-materialen worden gepresenteerd. Deze nemen de eerder vermelde nadelen weg die optraden bij de
klassieke aanpak voor het homogeniseren van materiaeiegenschappen. In de eerste methode, ook wel de discontinue homogenisatiemethode genoemd, wordt aangenomen dat het bulkmateriaal op macroniveau zich lineair-elastisch gedraagt. Hiervan worden de effectieve eigenschappen a-priori bepaald. Het gedrag van de cohesieve macroscheur komt echter voort uit ingebedde berekeningen die worden gedaan op onderliggende micromodellen (vergelijkbaar met FE² methoden). De methode is in staat om op een energetisch neutrale manier het op microschaal ontstane schadegebied te transformeren naar een cohesieve scheur op macroschaal. Door het a-priori aangenomen gedrag van het bulkmateriaal op macroschaal zijn de ingebedde microschaalberekeningen alleen nodig op plaatsen waar de macroscheur zich vormt of zich zal vormen. Dit maakt deze methode ten opzichte van de tweede methode minder rekenintensief.

De tweede NH aanpak die wordt gepresenteerd in dit proefschrift wordt ook wel als continu-discontinu aangeduid. In deze methode wordt zowel het gedrag van de cohesieve scheur, als ook het gedrag van het bulkmateriaal op macroschaal afgeleid van ingebedde micromodelsimulaties. Hoewel de continu-discontinu NH methode dus de rekenintensiefste is van de twee is hij als enige in staat om ook de energie die wordt gedissipeerd nog voor- dat er lokalistatie optreedt te modelleren.

Directe Numerieke Simulaties (DNS) worden gebruikt om beide methoden te verifiëren en om de numerieke efficiëntie aan te tonen van beide methoden zonder aan nauwkeurigheid in te boeten.

Gebruik makend van deze NH methoden wordt een raamwerk gepresenteerd voor het modelleren van materialen die zijn samengesteld uit heterogene lagen. Op macroniveau wordt een dergelijk materiaal geregenteerd door een serie interface-elementen waarvan de aanvankelijk elastische en cohesieve eigenschappen worden verkregen uit berekeningen aan micromodellen. Een nieuw schema wordt beschreven om het gekoppelde systeem van vergelijkingen (de evenwichtsvergelijkingen van het micromodel en de micro-macro transfervergelijkingen) op te lossen.

Als laatste wordt een volledig numeriek multischaal raamwerk gepresenteerd om het mechanische gedrag van uithardend cement te simuleren. Een drie-laags macro-meso-micromodel wordt uitgewerkt. Om de berekeningen uitvoerbaar te houden worden de berekeningen aan de micromodellen parallel uitgevoerd.
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V.P. NGUYEN

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Chapter 1

Introduction

1.1 Background

Many natural and engineering materials such as rock, concrete, metal, fiber-reinforced composites etc. have a heterogeneous structure at a certain level of observation, refer to Figure 1.1. These materials are often referred to as composite materials or multi-phase materials or heterogeneous materials. From an engineering point of view, composite materials are desirable because they can be tailor made to take advantage of particular properties of each constituent. For example, fiber reinforced concrete is concrete containing fibrous material in which fibres are usually used to control cracking.

![Figure 1.1 Scanning electron microscope (SEM) images of (a) concrete and (b) fiber reinforced composites.](image)

It has been widely recognized that many macroscopic phenomena originate from the mechanics of the underlying microstructure. The size, shape, spatial distribution, volume fraction and properties of the constituents making up the microstructure all have a significant impact on the behavior of the material observed at the macroscale. Furthermore, external loading applied on the materials at the macroscale might in turn cause changes in the microstructural morphology e.g., void formation and coalescence in metals, cracking in cement matrix and interfacial transition zone in concrete.

Finding the relation between microstructure and macroscopic properties (in short structure-properties relation) is an essential problem confronting
material scientists as well as the computational mechanics community for decades. Such relations, if found, might have a strong impact in many engineering fields. This is because (i) the macroscopic behavior is much better captured compared to a prediction based on phenomenological constitutive models and (ii) it provides an alternative to design new materials of which desired macroscopic properties can be fulfilled by adjusting the underlying microstructure. It is emphasized that the development of new materials is basically done empirically, that is, a large number of specimens with different microstructures are fabricated and tested, until specific requirements on the behavior are fulfilled. Obviously, computational models are preferable over this time consuming and expensive empirical method. Contribution to the on-going fundamental research in finding the structure-properties relations for quasi-brittle heterogeneous materials is one of the main objectives of this thesis.

Brute-force approaches in which the microstructure is explicitly taken into account at the coarse scale model are practically not feasible due to the prohibitive computational expense they would lead to. Therefore, over the years, a number of analytical/numerical models, that are usually referred to as multiscale models—models based on the physics of microstructures, which are able to predict, in an efficient manner, the macroscopic behaviour of heterogeneous materials—have been developed. Of particular interest are homogenization methods which allow one to substitute a heterogeneous material with an equivalent homogeneous material. In this thesis we confine to one particular homogenization theory, the computational homogenization theory, which has been proved to be an effective tool to perform scale bridging especially when the microstructure evolves in time (e.g., growth of micro-cracks) and is history-dependent. According to this method, a phenomenological constitutive model is not needed to describe the behaviour of the material at a macroscopic scale. Instead, the macroscopic solid is described by a homogenized effective constitutive law that is determined during the simulation based on the response of a microscopic sample where the heterogeneities of the microstructure are explicitly taken into account. Existing conventional homogenization models have, however, limited use for localization problems. When a softening material model is employed at the microscale, the homogenized stress-strain relation is a local strain softening constitutive equation. The consequence of this is that the macroscopic boundary value problem (BVP) becomes ill-posed, i.e. the macroscopic BVP loses ellipticity. This loss of ellipticity results in a sensitivity of the numerical
solution with respect to the macroscopic finite element discretization. Furthermore, for softening materials the response obtained with the bulk homogenization scheme is sensitive with respect to the size of the microscopic sample—the larger the microscopic sample the more brittle the homogenized response. A few extensions of conventional homogenization schemes have recently appeared in the literature which are able to deal with softening materials. However, they are developed specifically to some materials and thus not suitable to our target material—random heterogeneous materials exhibiting strain localization.

The objective of the research presented in this thesis is to develop a homogenization-based computational method to bridge failure mechanisms modelled at macroscale and microscale for quasi-brittle heterogeneous materials. Specific objectives are as follows

- Develop a homogenization technique by which the effective response is objective with respect to the size of the microscopic sample;
- Develop a computational homogenization method to model the transition from microscopic diffusive damage to macroscopic discrete cracking;
- Verify the developed models through comparisons against direct numerical simulations;
- Develop efficient algorithms so that multiscale crack simulations can be performed.

1.2 Scope and outline

The research presented in this dissertation falls within the category of computational solid mechanics. More precisely static equilibrium of a macroscopically homogeneous yet microscopically heterogeneous solid subjected to mechanical loadings is studied. The derivation is restricted to small displacement gradients in two dimensions. Furthermore, continuum mechanics is assumed to hold in all length scales involved. In this thesis, the terminology ‘multiscale’ should be understood as multiple length scales. The term ‘multiscale method’ indicates a formulation in which multiple length scales are treated separately and there is an exchange of information between the length scales.
Chapter 1 Introduction

The thesis is composed of nine chapters. The remainder of the thesis is organized as follows. In Chapter 2, numerical models that are used in subsequent chapters are discussed. Such models include (i) the finite element method (FEM) which is the basis of this work, (ii) the gradient enhanced damage model to resolve strain localization in a continuous framework and (iii) cohesive zone models together with the Partition of Unity method and interface elements to model discrete cracking. Also given in this chapter is a review of the state-of-the-art of multiscale modelling of heterogeneous materials.

Chapter 3 presents a numerical framework in which micromechanical modelling of concrete specimens can be performed. To this end, a numerical cement hydration model is implemented with which the microstructure of the cement paste that consists of unhydrated cement grains, hydration products and pores can be obtained. This numerical microstructure of cement paste is then discretized into finite elements upon which a damage model is applied to study the mechanical behavior of a hardening cement paste.

In Chapter 4, the concept of the representative volume element (RVE) for softening materials is revisited. It has been shown by many authors that by homogenizing towards a standard (local) stress-strain relation, there does not exist a microscopic sample which can be representative for softening materials. In this Chapter, we propose a new concept coined representative volume element for localization bands. A new averaging technique, the failure zone averaging scheme, is proposed with which it can be shown that a RVE does exist for softening materials. The confirmation of the existence of a RVE for materials that exhibit strain localization is an important ingredient for the homogenization-based multiscale models for localization problems to be developed in subsequent chapters.

From the result given in Chapter 4, in Chapter 5, a homogenization scheme for localization problems is developed. The main ingredients of the method are (i) the introduction of a cohesive crack at the macroscale, (ii) the behavior of that macro-crack is derived from finite element computations realized on a microscale sample in which all underlying heterogeneities are explicitly discretized and (iii) failure of the microscale sample is modelled with a continuum damage theory. The advantages of this model is that (i) it is insensitive to the macroscale/microscale finite element discretizations and (ii) it is objective with respect to the micro-sample size when this size is sufficiently large for random microstructures. Extension of the multiscale
cohesive crack model to the case of adhesive cracking i.e., cracking of the surface between two dissimilar materials, is also presented. To demonstrate the performance of the proposed models, some proof-of-concept numerical examples are given including a comparison with a direct numerical simulation.

In Chapter 6, the theory developed in Chapter 5 is further extended. Various issues including cyclic loading, crack propagation, treatment of snap-back in a multiscale simulation are presented. Also given in this Chapter are implementation aspects with a novel efficient technique to compute the macroscopic cohesive tangent matrix. The convergence characteristic of the proposed multiscale method is studied in detail. Numerical examples including propagation of curved cracks and comparison with a direct numerical simulation are given to demonstrate the capabilities of the method.

Chapter 7 presents a continuous-discontinuous computational homogenization scheme for modelling cohesive failure in random heterogeneous quasi-brittle materials. The scheme is a natural extension of the method described in Chapter 5 and 6 in which the mechanical behaviour of both macroscopic bulk and cohesive cracks are defined from nested microscopic finite element computations. Numerical examples are given to demonstrate the superiority of this continuous-discontinuous homogenization scheme to the original discontinuous homogenization method for problems that show diffusive damage beside a dominant localization band at the microscopic scale.

In Chapter 8, numerical models developed in previous chapters are utilized to devise a macro-meso-micro three scale model for concrete materials. A parallel implementation, to accelerate the computational time, of the multiscale model given in Chapter 5 is presented.

Chapter 9 ends the thesis by summarizing the key issues of the work presented in this dissertation and posting recommendations for future research.

1.3 Notations

The work presented in this dissertation involves continuum mechanics and numerical methods (e.g., FEM) each of them has its own standard notation. Therefore, three notations are adopted in this manuscript namely indicial notation, tensor notation and matrix notation (also known as engineering notation). Equations in continuum mechanics are written in indicial and tensor notation. Finite element formulations are expressed in matrix notation.
The squared magnitude of a three-dimensional vector expressed in three notations is given in the following equation

\[ r^2 = x_i x_i = \mathbf{x} \cdot \mathbf{x} = \mathbf{x}^T \mathbf{x} \]  \hspace{1cm} (1.1)

In indicial notation, the components of tensors are explicitly specified e.g., a vector in indicial notation is hence given by \( x_i \) in which the index \( i \) ranges from one to the number of spatial dimensions. Indices which are repeated twice in a term are summed, a rule known as the Einstein summation of which an example about the squared magnitude of a vector is as follows

\[ r^2 = x_i x_i = x_1^2 + x_2^2 + x_3^2 \]  \hspace{1cm} (1.2)

In tensor notation, tensors of order one or greater are written in boldface. Lower case bold-face letters are used for first-order tensors whereas upper case bold-face letters indicate high-order tensors, for example the symbol \( \mathbf{D} \) denotes the fourth-order elastic moduli tensor. The major exception to this rule are the physical stress tensor and the strain tensor which are second-order tensors, but are denoted by lower case symbols as \( \sigma \) and \( \epsilon \).

In matrix notation, the same symbols as for tensors are used to denote the matrices but the connective symbols (used to express the operators) are skipped. Symmetric high order tensors are expressed in matrix/vector forms using Voigt notation. For example, a two-dimensional stress tensor \( \sigma_{ij} \) is, in Voigt notation, written as a vector \( \begin{pmatrix} \sigma_{11}, \sigma_{22}, \sigma_{12} \end{pmatrix}^T \) and the fourth-order elastic moduli tensor \( \mathbf{D} \) is represented by a \( 3 \times 3 \) matrix \( \mathbf{D} \).

In this manuscript, subscripts \( \square_m \) and \( \square_M \) are used to indicate if a quantity belongs to the macroscale or microscale, respectively. Symbols are introduced at their first appearance. The term multiscale means multiple length scales.

### 1.4 Implementation

Numerical models presented in this dissertation (the gradient enhanced damage model, the phantom node model, the zero-thickness interface element model, the cement hydration model, the continuous CH model and the multiscale crack models) are implemented using the Jem/Jive C++ library [101]. Documentation of these computer codes is reported in [133].
Finite element meshes used in this thesis have been generated using two existing programs namely Gmsh [54] and SPACE [177]. SPACE, a discrete element package to simulate aggregated matter that is equipped with an unstructured meshing tool, was used to create meshes for the samples made of a heterogeneous random material. The remaining meshes were generated using Gmsh.
Chapter 2

Numerical modelling techniques for damage and fracture

This chapter briefly presents numerical methods/models that lay the foundation for the work given in this thesis. The finite element method, that is the general numerical framework employed here, is briefly given in Section 2.1. Strain localization phenomena and relevant numerical models are presented in Section 2.2. Continuous approaches that employ generalized constitutive models and discontinuous formulations, in which a jump in the displacement field is allowed, are reviewed. Latest numerical methods dealing with strain localization problems are presented. Multiscale modelling of heterogeneous materials is a topic discussed in Section 2.3. Section 2.4 presents the basic ingredients of the continuous computational homogenization method for homogenization towards a stress-strain law for the macroscopic bulk material. Existing schemes for homogenization towards a cohesive law (the discontinuous computational homogenization method) are given in Section 2.5. In this chapter, an overview of the state-of-the-art of multiscale modelling of inelastic heterogeneous materials is given with emphasis on computational homogenization methods.

2.1 The finite element method

The work in this thesis is based on the finite element method (FEM) which is a powerful method to numerically solve a wide range of partial differential equations governing various physical phenomena. There are excellent textbooks on this subject [14, 74]. The aim of this section is to present a short introduction to this field in the context of inelastic deformable solids subjecting to a quasi-static mechanical excitation.

Considering a solid $\Omega$, as shown in Figure 2.1, that is bounded by $\Gamma$. Prescribed displacements $\bar{u}$ are imposed on the Dirichlet boundary $\Gamma_u \subseteq \Gamma$ and prescribed tractions $\bar{t}$ are applied on the Neumann boundary $\Gamma_t \subseteq \Gamma$.

The problem is to find a displacement field $u$ that satisfies the following governing equations
Figure 2.1 A two-dimensional body subject to a traction \( \mathbf{t} \), a body force \( \mathbf{b} \) and an imposed displacement \( \mathbf{\bar{u}} \).

\[ \nabla \cdot \sigma + \mathbf{b} = 0 \quad \text{in } \Omega \]  
\[ \mathbf{e} = \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \]  
\[ \sigma = f(\mathbf{e}, \alpha) \]  
\[ \sigma \cdot \mathbf{n} = \mathbf{t} \quad \text{on } \Gamma_t \]  
\[ \mathbf{u} = \mathbf{\bar{u}} \quad \text{on } \Gamma_u \]  

where \( \sigma \) is the second order Cauchy stress tensor, \( \mathbf{b} \) is the body force vector and \( \mathbf{e} \) is the strain tensor; \( \nabla, \nabla, T \) denote the divergence, gradient and transpose operators, respectively. In the above, Equation (2.1a) is the equilibrium equation, Equation (2.1b) is the kinematic equation, Equation (2.1c) is the constitutive equation with \( \alpha \) being the so-called internal variables. The two last equations denote the boundary conditions and \( \mathbf{n} \) is the outward unit normal vector on \( \Gamma_t \).

The FEM is based on the following weak form: find the displacement field \( \mathbf{u} \) such that

\[ \int_\Omega \mathbf{e}^T (\delta \mathbf{v}) \sigma (\mathbf{u}) d\Omega = \int_\Omega \delta \mathbf{v}^T \mathbf{b} d\Omega + \int_{\Gamma_t} \delta \mathbf{v}^T \mathbf{t} d\Gamma \]  

for all \( \delta \mathbf{v} \) that is sufficiently smooth so that all operations in which they are involved make sense. For a rigorous discussion on the function space in FEM, we refer to [74]. In the above, the vector \( \delta \mathbf{v} \) represents the so-called virtual displacements.
The spatial domain $\Omega$ is discretized into $n_e$ elements (with simple geometry) of which vertices are called nodes. A typical finite element mesh with three-noded triangular elements is given in Figure 2.2. Associated to each node $I$ is a shape function or interpolation function $N_I(x)$ which has a compact support i.e., $N_I(x)$ is nonzero only over elements sharing node $I$.

In each element the displacement field as well as the virtual displacement field are approximated by the shape functions $N_I(x)$ associated with the nodes of that element

$$u_e(x) = N(x) a_e \quad (2.3a)$$
$$\delta v_e(x) = N(x) \delta a_e \quad (2.3b)$$

where $N$ denotes the matrix of shape functions, $a_e = [a_{1x}^1, a_{1y}^1, \cdots, a_{nx}^n, a_{ny}^n]^T$ is the vector of nodal displacements of element $e$ and $x$ denotes the spatial coordinates. The number of nodes per element is $nn$.

Using Equation (2.1b), the strain inside element $e$ is given by

$$e_e(u) = B_e a_e, \quad e_e(\delta v) = B_e \delta a_e \quad (2.4)$$

where $B_e$ is the strain-displacement matrix defined as $B_e = [B_1, B_2, \ldots, B_{nn}]$ with $B_I$ being given by

$$B_I = \begin{bmatrix} N_{Ix} & 0 & N_{Iy} \\ 0 & N_{Ix} & 0 \\ N_{Iy} & N_{Ix} & \end{bmatrix} \quad (2.5)$$

---

**Figure 2.2** Finite element mesh in two dimensions.
Chapter 2 Numerical modelling techniques for damage and fracture

where a comma denotes differentiation with respect to the variable which follows.

The integral over \( \Omega \) in the weak form, Equation (2.2), is computed as a sum of integrals over element domains \( \Omega_e \). Substituting Equations (2.3) and (2.4) into the weak form (2.2) yields

\[
\sum_{e=1}^{n_e} \left( \int_{\Omega_e} \delta \mathbf{a}_e^T \mathbf{B}_e^T \sigma_e \, d\Omega \right) = \sum_{e=1}^{n_e} \left( \int_{\Omega_e} \delta \mathbf{a}_e^T \mathbf{N}_e^T \mathbf{b}_e \, d\Omega \right) + \sum_{e=1}^{n_e} \left( \int_{\Gamma_e} \delta \mathbf{a}_e^T \mathbf{N}_e^T \mathbf{t}_e \, d\Gamma \right)
\]

(2.6)

The displacements of all nodes of the mesh are collected in one large vector \( \mathbf{a} \), the global nodal displacements vector. The elementary nodal displacements vector and the global nodal displacements vector are related via

\[
\mathbf{a}_e = \mathbf{L}_e \mathbf{a}
\]

(2.7)

with \( \mathbf{L}_e \) being the location matrix which is a sparse, boolean matrix containing only 0 and 1. Similarly, one writes \( \delta \mathbf{a}_e = \mathbf{L}_e \delta \mathbf{a} \). With this, Equation (2.6) becomes

\[
\sum_{e=1}^{n_e} \left( \int_{\Omega_e} \delta \mathbf{a}_e^T \mathbf{L}_e^T \mathbf{B}_e^T \sigma_e \, d\Omega \right) = \sum_{e=1}^{n_e} \left( \int_{\Omega_e} \delta \mathbf{a}_e^T \mathbf{L}_e^T \mathbf{N}_e^T \mathbf{b}_e \, d\Omega \right) + \sum_{e=1}^{n_e} \left( \int_{\Gamma_e} \delta \mathbf{a}_e^T \mathbf{L}_e^T \mathbf{N}_e^T \mathbf{t}_e \, d\Gamma \right)
\]

(2.8)

Since the above holds for any \( \delta \mathbf{a} \), one obtains

\[
\sum_{e=1}^{n_e} \left( \mathbf{L}_e^T \int_{\Omega_e} \mathbf{B}_e^T \sigma \, d\Omega \right) = \sum_{e=1}^{n_e} \left( \mathbf{L}_e^T \int_{\Omega_e} \mathbf{N}_e^T \mathbf{b} \, d\Omega \right) + \sum_{e=1}^{n_e} \left( \mathbf{L}_e^T \int_{\Gamma_e} \mathbf{N}_e^T \mathbf{t} \, d\Gamma \right)
\]

(2.9)

or equivalently

\[
\mathbf{f}_{\text{int}}(\mathbf{a}) = \mathbf{f}_{\text{ext}}
\]

(2.10)

where \( \mathbf{f}_{\text{int}} \) and \( \mathbf{f}_{\text{ext}} \) are the internal force vector and external force vector, respectively. They are given by
2.2 Strain localization and modelling approaches

\[
f_{\text{int}} = \sum_{e=1}^{n_e} L_e^{T} \left( \int_{\Omega_e} B_e^{T} \sigma_e d\Omega \right)
\]  \hspace{1cm} (2.11a)

\[
f_{\text{ext}} = \sum_{e=1}^{n_e} L_e^{T} \left( \int_{\Omega_e} N_e^{T} b_e d\Omega + \int_{\Gamma_e} N_e^{T} t_e d\Gamma \right)
\]  \hspace{1cm} (2.11b)

The internal and external nodal force vectors are computed by looping over all elements, for each element the elementary quantity \( \int_{\Omega_e} (\cdot) d\Omega \) is determined and assembled to the corresponding global quantity using the location matrix \( L_e \).

For a given external force vector, the highly nonlinear Equation (2.10) is solved iteratively using the Newton-Raphson method (see e.g., [33] for details). The displacement at iteration \( i + 1 (a_{i+1}) \) is obtained from the displacement at the previous iteration \( i (a_i) \) as follows

\[
a_{i+1} = a_i + \Delta a_i, \quad \Delta a_i = K^{-1} r, \quad r = f_{\text{ext}} - f_{\text{int},i}
\]  \hspace{1cm} (2.12)

the process is repeated until \( a_{i+1} \) is close enough to \( a_i \). Solution of the linear equation \( \Delta a_i = K^{-1} r \) is obtained with a linear solver which can be a direct solver (e.g., a direct frontal solver) or an iterative solver (e.g., the Preconditioned Conjugate Gradient solver). In the above, \( r \) is the residual vector and \( K \) denotes the stiffness matrix which is given by

\[
K = \frac{\partial f_{\text{int}}}{\partial u} = \sum_{e=1}^{n_e} L_e^{T} \left( \int_{\Omega_e} B_e^{T} D \sigma_e d\Omega \right) L_e
\]  \hspace{1cm} (2.13)

where \( D \) is the material tangent, a fourth order tensor, that relates the strain rate to the stress rate i.e., \( \dot{\sigma} = D \dot{e} \). The integral of elementary quantities \( \int_{\Omega_e} (\cdot) d\Omega \) is computed numerically using a quadrature rule e.g., a Gauss rule.

For softening materials, the complete static equilibrium path can only be traced using a displacement control or an arc-length control. We refer to [34, 38, 51] for details.

2.2 Strain localization and modelling approaches

Many materials show a gradual decrease of their load-carrying capacity when deformed beyond a certain limit. Such materials are called softening
Chapter 2 Numerical modelling techniques for damage and fracture

materials. When subjected to extreme loading conditions, specimens made of a softening material exhibit strain localization i.e., the strain is concentrated in narrow bands while the rest of the specimen experiences unloading. For a detailed description on strain localization, the reader is referred to [169].

Basically, there are three approaches to modelling strain localization problems namely (i) the continuous approach, (ii) the discontinuous approach and (iii) the continuous-discontinuous approach. As the name implies, in continuous approaches, the displacement field is continuous. On the contrary, the displacement field can exhibit a jump across a plane i.e., a crack can be modelled according to discontinuous approaches. In the continuous-discontinuous technique, which is a combination of the continuous and discontinuous modelling strategies, the early stage of failure is modelled with a continuous model and the final stage of failure is dealt with by inserting a traction-free crack [167, 168]. In [128], a novel cohesive zone model has been devised by which the transition from initial diffusive damage to final discrete cracks in porous media can be achieved. Figure 2.3 shows an example of modelling of failure of concrete structures with a continuous and a discontinuous approach.

![Figure 2.3 Failure modelling of a concrete beam with continuous approach (left) and discontinuous approach (right).](image)

Remark 2.2.1. In the field of concrete fracture mechanics, yet another approach which is called the lattice model, see e.g., [36, 64, 160] has become more popular. According to lattice models, a concrete sample is discretized by a network of beam or truss elements. The heterogeneity of concrete is obtained by overlaying a mesostructure on top of the lattice. Fracture can then be modelled by removing, from the lattice, the beam (or truss) elements in which the maximum stress exceeds the critical stress.
2.2 Strain localization and modelling approaches

2.2.1 Continuous approaches

Modelling strain localization in the framework of continuous approaches rely on the so-called generalized models which are generalization of the classical continuum theory. That is because classical continuum models (also known as local models), i.e. continuum models that do not incorporate an internal length scale, suffer from excessive mesh dependence in numerical analyses of localization problems. Generalized continua can be continua with microstructure e.g., a Cosserat-type continua [22] or continua with generalized constitutive equations. Notable examples of generalized constitutive models include the non-local continuum theory [7, 9, 154], the gradient-dependent plasticity model [21, 23], the gradient enhanced damage model [52, 150] and the plastic-damage model see e.g., [62, 63]. Recently, a new objective approach coined the thick level set method has been proposed in [126] to model damage growth in solids. The common characteristic of these methods is the presence of an internal length scale in the formulation. Another regularization method is the viscous regularization approach [164]. In this thesis, the gradient enhanced damage formulation [150] is adopted to model failure at the microscale. For sake of completeness, this model is summarized here.

Material degradation is modelled by a simple isotropic damage model. The stress-strain relation is given by [98]

\[
\sigma = (1 - \omega)D : \varepsilon
\]  

where \( \omega \) is the scalar damage variable \( (0 \leq \omega \leq 1) \) and the fourth order tensor \( D \) contains the elastic moduli.

Damage can be governed by the following exponential law [113]

\[
\omega = \begin{cases} 
0 & \text{if } \kappa \leq \kappa_l \\
1 - \frac{\kappa}{\kappa_l} \left[1 - \gamma + \gamma \exp^{-\beta(\kappa - \kappa_l)}\right] & \text{if } \kappa > \kappa_l 
\end{cases}
\]  

where \( \gamma \) (residual stress), \( \beta \) (softening slope) and \( \kappa_l \) (damage threshold) denote the inelastic parameters. The variable \( \kappa \) is a scalar measure of the largest strain ever reached which is defined via the following loading function \( f \)

\[
f = \bar{\varepsilon}_{eq} - \kappa
\]
that subjects to the equivalent Kuhn-Tucker condition stated as

\[ \dot{\kappa} \geq 0, \quad f \leq 0, \quad \dot{\kappa} f = 0 \]  

(2.17)

Note that \( f \) specifies the elastic domain i.e., the set of states for which damage does not occur. Its role is similar to the yield function in flow theory of plasticity.

In Equation (2.16), \( \tilde{\varepsilon}_{eq} \) is the nonlocal equivalent strain which is, according to the gradient enhanced model [150], given by

\[
\frac{\tilde{\varepsilon}_{eq} - c \nabla^2 \tilde{\varepsilon}_{eq}}{\nabla \tilde{\varepsilon}_{eq} \cdot \mathbf{n}} = \varepsilon_{eq} \quad \text{in } \Omega \\
\nabla \tilde{\varepsilon}_{eq} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma
\]  

(2.18)

where \( c \) denotes a positive parameter of the dimension length squared. The second equation in Equation (2.18) is the boundary conditions of the nonlocal equivalent strain field that ensures that, for a homogeneous deformation state, \( \tilde{\varepsilon}_{eq} \) equals \( \varepsilon_{eq} \). The local equivalent strain \( \varepsilon_{eq} \) is, for tensile failure in two dimensions studied in this work, defined as [113]

\[
\varepsilon_{eq} = \sqrt{\langle \varepsilon_1 \rangle^2 + \langle \varepsilon_2 \rangle^2}
\]  

(2.19)

where \( \varepsilon_i \) represents the principal strain and the Macauley’s brackets \( \langle x \rangle \) denote the positive part of \( x \).

The finite element discrete equations read

\[
\int_{\Omega} B^T \sigma \, d\Omega = f^{ext} \quad \text{(2.20a)}
\]

\[
\int_{\Omega} N_e^T \varepsilon_{eq} \, d\Omega + \int_{\Omega} B^T_e \varepsilon_{eq} \, d\Omega = \int_{\Omega} N_{eq} \varepsilon_{eq} \, d\Omega \quad \text{(2.20b)}
\]

where \( N_e \) denotes the vector containing shape functions used to discretized the scalar field \( \tilde{\varepsilon}_{eq} \) and \( B_e = \nabla N_e \).

Details on the gradient enhanced damage model can be found in [149, 166].
2.2 Strain localization and modelling approaches

2.2.2 Discontinuous approaches

The first discontinuous model for strain localization in concrete has been presented in [72] using the cohesive zone model [4, 42]. In cohesive zone models, the inelastic deformation ahead of the crack tip is modelled by cohesive forces acting on a fictitious extension of the crack. Therefore, two constitutive equations are needed in describing a solid with cohesive cracks namely the standard constitutive equation for the bulk material, see Equation (2.1c), and a cohesive law (also known as a traction-separation law) that relates the crack opening $\|u\|$ to the cohesive force $t$

$$t = g(\|u\|, \beta)$$  \hspace{1cm} (2.21)

where $\beta$ represents some internal variables characterizing the irreversibility of the failure phenomenon.

![Figure 2.4](initially_elastic_tsl_initially_rigid_tsl.png)

**Figure 2.4** Two commonly used traction-separation laws (TSL).

There are two classes of cohesive laws namely (i) initially elastic cohesive laws and (ii) initially rigid cohesive laws. Two typical representatives of those traction-separation laws (TSLs) are given in Figure 2.4. The former are most often used to model debonding of the interface between two materials because they allow the hardening regime prior to debonding to be included. The latter are adopted to model cohesive cracking in the bulk material. Note that initially rigid cohesive laws must be used in combination with a separate failure criterion for the initiation of failure due to the lack of an inherent damage initiation criterion in the TSL. For this reason, they are referred to as *extrinsic* cohesive models according to [90]. Initially elastic cohesive models are known as *intrinsic* cohesive models.
Cohesive laws are characterized by two key parameters namely the tensile strength $f_t$ and the fracture energy $G_{Ic}$. They are considered as material properties and determined by the so-called parameter identification processes which can rely solely on experimental tests, see for instance [162] or a combined experimental-numerical framework [32] centred on inverse analysis [27]. Cohesive laws as given in Equation (2.21) are referred to as phenomenological cohesive laws. A review on cohesive zone models is given in [45].

In order to ensure the quadratic convergence property of the Newton-Raphson method the above cohesive law is usually cast into rate form as $\dot{t} = T[\dot{u}]$ in which $T$, a second order tensor, is the so-called (consistent) cohesive tangent which is given by $T = \frac{\partial t}{\partial [u]}$.

The biggest challenge in using cohesive zone models in the FEM framework is how to resolve the displacement discontinuity. The earliest solution is using zero-thickness interface elements [143, 186, 202]. Since interface elements are placed along the inter-element boundaries prior to the simulation, the simulated fracture pattern suffers to a certain extent from the mesh bias. However these elements find good applications for problems in which the crack path is known a priori e.g., delamination in a composite material, see Figure 2.5. Elements with embedded discontinuities [3, 100, 142, 165, 197] provide a way to introduce the discontinuity inside the element. An advantage of this method is that it can be easily incorporated into existing finite element codes. Adaptive remeshing techniques are also utilized, predominantly in industry, to model traction-free cracks, see [24, 25] and references therein.

Nowadays, the Partition of Unity Method (PUM) is probably the most frequently used numerical method for modelling discontinuities in the FEM
framework. Early applications of PUM found in the field of Linear Elastic Fracture Mechanics (LEFM) [12, 124] in which the authors proposed the name eXtended Finite Element Method (XFEM). Modelling cohesive cracks using PUM has been given in [123, 198]. For a comprehensive review of PUM, see [50]. Implementation of PUM in existing finite element packages is however not straightforward. The issue of computer implementation of PUM has been presented in [20, 57, 179]. A review on numerical aspects of cohesive zone models has been given in [39].

For completeness, crack modelling has also been treated with other methods notably meshfree methods, see among others [37, 111, 155, 156] and references therein. Recently, an isogeometric approach [76] to cohesive zone modelling has been presented in [195]. Yet another interesting method for fracture modelling is the recently emerged phase field based model of fracture [122]. The Boundary Element Method (BEM) of which a classic can be found in [26], is also utilized to model cohesive crack growth [203]. Peridynamics model* (see e.g., [163]) is another approach for crack modelling. A comparative study of XFEM and peridynamics for modelling dynamics fracture is given in [1].

In this work, interface elements are utilized to model heterogeneous material layers whereas PUM is adopted to simulate propagation of cohesive cracks. For this reason, a brief introduction to PUM and interface elements is given in what follows.

**Partition of Unity Method**

Partition of Unity FEM (PUFEM) [114] allows an arbitrary function \( \Phi(x) \) to be incorporated into the standard finite element solution space according to

\[
\mathbf{u}^h(x) = \sum_{I \in S} N_I(x) \mathbf{u}_I + \sum_{J \in S_{\text{enr}}} N_J(x) \Phi(x) \mathbf{a}_J 
\]  

(2.22)

where \( S \) denotes the set of nodes and \( S_{\text{enr}} \) is the set of enriched nodes. The additional nodal unknowns are represented by \( \mathbf{a} \). Since \( \Phi(x) \) is added to enrich the standard finite element solution space, it is called an enrichment function.

*The peridynamic theory is based on integral equations, in contrast with the classical theory of continuum mechanics, which is based on partial differential equations.
For a body $\Omega$ crossed by a crack $\Gamma_d$ into two parts $\Omega^+$ and $\Omega^-$, see Figure 2.6, the displacement field is discontinuous across $\Gamma_d$. The enrichment function is therefore the Heaviside function $H(x)$ which is given by

$$H(x) = \begin{cases} 1 & x \in \Omega^+ \\ 0 & x \in \Omega^- \end{cases} \quad (2.23)$$

The displacement field is thus given by [12, 124]

$$u^h(x) = \sum_{I \in S} N_I(x) u_I + \sum_{J \in S_{enr}} N_J(x) H(x) a_J \quad (2.24)$$

where $S_{enr}$ contains nodes whose support is cut by the crack $\Gamma_d$, see Figure 2.7.

The phantom node method In [118] the authors presented a method in which a cracked element is modelled as a pair of overlapping elements, see Figure 2.8. This method has been shown later to be equivalent to the XFEM with Heaviside enrichment in [172].
2.2 Strain localization and modelling approaches

The phantom node method: replacing a cracked element by a pair of two overlapping elements. Filled circle nodes are existing standard nodes whereas circle nodes are the added phantom nodes.

The displacement field inside a cracked element (replaced by two overlapping elements) is given by

\[
\mathbf{u}(x) = \begin{cases} 
\mathbf{N}(x)a_A & x \in \Omega_A \\
\mathbf{N}(x)a_B & x \in \Omega_B 
\end{cases} 
\]  

where \(a_A\) and \(a_B\) denote the nodal displacements of element A and B, respectively.

The displacement jump is given by

\[
\llbracket \mathbf{u} \rrbracket(x) = \mathbf{N}(x)(a_A - a_B) \quad x \in \Gamma_d 
\]  

The variation of the displacement jump is thus defined as

\[
\delta \llbracket \mathbf{v} \rrbracket(x) = \mathbf{N}(x)(\delta a_A - \delta a_B) 
\]  

One attractive property of PUM is that only the standard variational equation needs be considered with the displacement field being the only independent unknown field. For cohesive cracks, this variational equation reads

\[
\int_{\Omega} e^T(\delta \mathbf{v}) \sigma (\mathbf{u}) \, d\Omega = \int_{\Omega} \delta \mathbf{v}^T \mathbf{b} \, d\Omega + \int_{\Gamma_d} \delta \mathbf{v}^T \mathbf{t} \, d\Gamma - \int_{\Gamma_d} \delta [\mathbf{v}]^T \mathbf{t} \, d\Gamma 
\]

which is exactly the weak form given in Equation (2.2) added by a term representing the virtual work done by the cohesive force (the third term of the RHS of the above).
Substituting Equations (2.3), (2.4) and (2.27) into Equation (2.28) yields the following discrete equation

\[ f_{\text{ext}} = f_{\text{int}} \equiv f_{\text{bulk}} + f_{\text{coh}} \]  

(2.29)

where the bulk force vector \( f_{\text{bulk}} \) and the cohesive force vector \( f_{\text{coh}} \) for a pair of elements \( A \) and \( B \) are given by

\[ f_{A,\text{bulk}} = \int_{\Omega_A} B^T \sigma d\Omega, \quad f_{B,\text{bulk}} = \int_{\Omega_B} B^T \sigma d\Omega \]  

(2.30)

\[ f_{A,\text{coh}} = \int_{\Gamma_d} N^T t d\Gamma, \quad f_{B,\text{coh}} = -\int_{\Gamma_d} N^T t d\Gamma \]  

(2.31)

The linearized system of equations then reads

\[
\begin{pmatrix}
K_A & 0 \\
0 & K_B
\end{pmatrix}
+ 
\begin{pmatrix}
-K_{\text{coh}} & -K_{\text{coh}} \\
-K_{\text{coh}} & K_{\text{coh}}
\end{pmatrix}
\begin{pmatrix}
\Delta a_A \\
\Delta a_B
\end{pmatrix}
= 
\begin{pmatrix}
\delta f^A_{\text{int}} \\
\delta f^B_{\text{int}}
\end{pmatrix}
- f_{\text{ext}}
\]  

(2.32)

with the bulk stiffness matrix and the cohesive stiffness matrix being given by

\[ K_I = \int_{\Omega_i} B^T DB d\Omega, \quad I = A, B \]  

(2.33)

\[ K_{\text{coh}} = \int_{\Gamma_d} N^T TN d\Gamma \]  

(2.34)

**Zero-thickness interface elements**

For a comprehensive treatment of the interface element formulation, we refer to, among others, [10, 143, 158, 202] and references therein. Here the basics of the method are illustrated by considering the four-node linear interface element shown in Figure 2.9, the displacement of its upper and lower surfaces is given by

\[ u^+ = N_1 a^+_1 + N_2 a^+_2, \quad u^- = N_1 a^-_1 + N_2 a^-_2 \]  

(2.35)

with \( N_1, N_2 \) the shape functions of the two-node line elements and \( a^+_i \) and \( a^-_i (i = 1, 2) \) denote the nodal displacements of the upper face and lower face, respectively.
2.2 Strain localization and modelling approaches

Figure 2.9 Four-noded linear interface elements placed along the inter-element boundaries to model a crack.

Having defined the displacement of the upper and lower faces of the interface, the displacement jump can be computed according to

\[
[u(x)] = u^+ - u^- = N_{\text{int}}(a^+ - a^-) \tag{2.36}
\]

where use was made of Equation (2.35). In the above, \(N_{\text{int}}\) is given by

\[
N_{\text{int}} = \begin{bmatrix} N_1 & 0 & N_2 & 0 \\ 0 & N_1 & 0 & N_2 \end{bmatrix} \tag{2.37}
\]

and \(a^+ = [a_{1x}^+, a_{1y}^+, a_{2x}^+, a_{2y}^+]^T\). A similar definition for \(a^-\) can be defined.

The cohesive force vector is computed by assembling the contribution of all interface elements. It is given by for an interface element \(ie\)

\[
f_{ie,+,\text{coh}} = + \int_{\Gamma_4} N_{\text{int}}^T \mathbf{t} d\Gamma, \quad f_{ie,,-,\text{coh}} = - \int_{\Gamma_4} N_{\text{int}}^T \mathbf{t} d\Gamma \tag{2.38}
\]

where \(f_{ie,+,\text{coh}} / f_{ie,,-,\text{coh}}\) is assembled to \(f_{\text{int}}\) according to the degrees of freedom (dofs) of nodes of the upper/lower surfaces.

The tangent stiffness matrix of an interface element \(ie\) is given by

\[
K_{ie}^{\text{int}} = \begin{bmatrix} \int_{\Gamma_4} N_{\text{int}}^T \mathbf{N} N_{\text{int}} d\Gamma & - \int_{\Gamma_4} N_{\text{int}}^T \mathbf{N} N_{\text{int}} d\Gamma \\ - \int_{\Gamma_4} N_{\text{int}}^T \mathbf{N} N_{\text{int}} d\Gamma & \int_{\Gamma_4} N_{\text{int}}^T \mathbf{N} N_{\text{int}} d\Gamma \end{bmatrix} \tag{2.39}
\]
Integration along the interface elements \( \int_{\Gamma} (\cdot) d\Gamma \) is performed with a nodal integration scheme (lowest order Newton-Cotes rule) to avoid oscillations in the traction profile \[158\]. Obviously implementation of interface elements is straightforward provided a mesh with duplicated nodes. The topic of modifying a FE mesh to insert interface elements has not been discussed in literature and no free interface element generator program is publicly available. In \[131\], such a program is described.

2.3 Multiscale modelling of heterogeneous materials

Traditionally multiscale modelling of heterogeneous materials is performed either within the framework of *homogenization methods* for problems in which the scales are clearly separated or within the framework of *concurrent methods* when the scales are coupled. This section gives an overview of the state-of-the-art of these two theories with emphasis on homogenization methods which are pursued in this research. The discussion is restricted to continuum/continuum coupling. For atomistic/continuum coupling i.e., MD-FEM coupling, refer to an overview reported in \[35\] and for discrete/continuum coupling i.e., DEM-FEM coupling, see \[196\] and references therein where MD stands for molecular dynamics and DEM is short for discrete element method.

2.3.1 Homogenization methods

Homogenization is a method to determine the *apparent* or *overall* properties of a heterogeneous material thereby allowing one to substitute this material with an equivalent homogeneous material, see Figure 2.10. Homogenization methods can be divided into three categories namely analytical/mathematical homogenization, numerical homogenization and computational homogenization. In this thesis, analytical homogenization, albeit very useful in some circumstances, is left out of consideration since this technique is usually restricted to simple microscopic geometries and material models (often linear elastic). A comprehensive overview of analytical homogenization methods can be found in the textbook \[130\].

In numerical homogenization schemes, a macroscopic canonical constitutive model e.g., a visco-plasticity model, is assumed with parameters determined by fitting the data produced by FE (or any other numerical method) computations of a microscopic sample where the microstructure is explicitly
2.3 Multiscale modelling of heterogeneous materials

Homogenization of a heterogeneous material. Based on [184].

Figure 2.10 Homogenization of a heterogeneous material. Based on [184].

modelled. In the literature, those numerical homogenization techniques are known as unit cell methods, refer to [29, 192] among others and references therein. Due to the assumption on the form of the macroscopic constitutive law, the methods become less appropriate for highly nonlinear problems. On the other hand, these methods are computationally attractive for large scale computations since microscopic FE computations are conducted \textit{a priori}.

According to computational homogenization methods [181], the macroscopic constitutive behavior is defined \textit{on the fly} during the simulation. Due to this flexibility, these methods have been utilized to predict mechanical behavior of materials having complex microstructures, see [55, 65, 86, 121, 170] among others. Not only mechanical problems describing linear and nonlinear deformations but also thermal problems [95, 127, 146] and multi-physics (thermo-mechanical) problems [147] have recently been addressed by this method. Other applications encompass thin structures [30, 116, 117, 144, 145] and uncoupled consolidation in heterogeneous porous media [94]. A unified variational basis of CH theory for bulk materials has been recently presented in [152]. A review of CH methods and applications has been given in [53].

In [187, 188] a homogenization scheme using an artificial neural network (ANN) was presented. The basic idea is to combine the numerical homogenization (efficient but restricted) and computational homogenization (gen-
eral but expensive) into one common framework. To this end, an ANN is used as a material model on the macroscale. The ANN is trained using microscale simulations.

### 2.3.2 Concurrent methods

The characteristic of concurrent methods is that the microstructural features are resolved directly on the macroscopic model. Two basic issues involved in this kind of method are (i) how to handle the coupling between the coarse mesh and the fine mesh and (ii) efficient algorithms for adaptive addition of fine scale features to the coarse scale model. Typical works are [44, 66, 102] which are based on domain decomposition methods and [69, 104] which are based on the variational multiscale method [75]. Figure 2.11 gives some concurrent models for failure analysis of heterogeneous materials. Another multiscale method with strong macro-micro coupling has been given in [78] for elasto-plastic multiphase materials and in [59] for quasi-brittle softening materials. Multiscale methods that adaptively combine a (numerical) homogenization technique and a concurrent method have been presented in, among others, [56, 93, 183] and references therein. A homogenized constitutive model (obtained via a numerical homogenization) is utilized for domains having benign deformations while a concurrent formulation is adopted in critical regions of high gradients where the macroscopic fields vary considerably. A numerical multiscale method for modelling fracture of heterogeneous quasi-brittle solids has been given in [82] where the designation *numerical* is used to indicate the use of a multi-grid solution strategy to solve the very large system of algebraic equations that emerges from detailed resolution of the fine-scale structure. This method can be viewed as a Direct Numerical Solution (DNS) with an efficient solution scheme.

### 2.4 Continuous computational homogenization model

This section briefly presents the continuous computational homogenization method. Through this, basic concepts of CH methods are discussed. The material given in this section is required in developing enhanced discontinuous and continuous-discontinuous CH schemes, to be presented in subsequent chapters, for strain localization and failure phenomena.
2.4 Continuous computational homogenization model

Continuous computational homogenization (CH) methods are utilized to define on the fly the macroscopic stress-strain relation $\sigma_M - \epsilon_M$ for a macroscopic point from a microscopic sample attached to this point. That is why CH is also referred to as multiscale constitutive modelling. All the heterogeneities of the underlying microstructure are explicitly resolved in the microscopic sample. The behavior of the microstructural constituents are modelled by a classic phenomenological constitutive law. The procedure is given in Figure 2.12 which can be briefly described as follows. For a point (e.g., an integration point in the spatially discretized macroscopic solid) in the macro-solid with a strain $\epsilon_M$, instead of inserting this strain into a (phenomenological) constitutive box to obtain the corresponding stress $\sigma_M$, the strain is used as a boundary condition imposed on the external boundary $\Gamma_m$ of the microscopic sample $\Omega_m$. The equilibrium of this micro-sample is obtained after solving the microscopic boundary value problem (BVP).

![Figure 2.11](image-url)

*Figure 2.11* Concurrent multiscale models based on: (a) overlapping domain decomposition method [44] and (b) variational multiscale method [69].
Figure 2.12 Multiscale modelling of a heterogeneous solid with the continuous/bulk computational homogenization scheme.

The macroscopic stresses $\sigma_M$ are then defined as the volume average of the microscopic stresses over the micro-sample. When implemented in a finite element (FE) framework, the method is known as an FE$^2$ [47] scheme or, more generally, a multilevel FEM. The discussion here is confined to two-dimensional quasi-static problems. For a treatment of computational homogenization in a three-dimensional dynamic setting, we refer to [83, 199]. A two-dimensional multiscale method for impact modelling of viscoelastic solids having a random microstructure that contains a field of evolving microcracks has been given in [173]. A comprehensive treatment of CH theory in the finite deformation regime is given in the dissertation [85].

2.4.2 Basic ingredients of CH theory

The theory of homogenization is based on the following ingredients

- Existence of a Representative Volume Element (RVE)
- Principle of separation of scales
2.4 Continuous computational homogenization model

- Averaging theorem e.g., strain and stress averaging theorems
- The Hill-Mandel macro-homogeneity principle
- Availability of constitutive behaviour of RVE’s constituents

The concept and the issue of existence of the RVE will be discussed later. For the subsequent discussion an assumption was made of the existence of such a RVE. In the following discussion, it has been assumed that the RVE does not contain cracks. Furthermore, voids, if present in the RVE, are traction-free i.e., the traction vanishes on the surfaces of the voids. Relaxation of the first assumption was made in [205] whereas the extension of the CH theory to the case in which second assumption is relaxed has been given in [152].

**Principle of separation of scales**

According to [53], the principle of separation of scales is formulated as follows: “The microscopic length scale \( l_m \) is assumed to be much smaller than the characteristic length \( l_M \) over which the macroscopic loading varies in space”. That is,

\[
 l_m \ll l_M \quad (2.40)
\]

which requires the RVE to be sufficiently small so that the macroscopic strain is uniform over it. Since the volume \( \Omega_m = \mathcal{O}(l_m^3) \), the inertial and body forces can be neglected at the microscale. Therefore the general dynamic equilibrium of the RVE reduces to the static equilibrium that reads

\[
 \nabla \cdot \sigma_m = 0 \quad \text{in} \ \Omega_m \quad (2.41)
\]

**Strain averaging theorem**

The strain at any point \( x_M \) in the macroscopic solid is defined as the volume average of the microscopic strain \( \epsilon_m \) over the RVE that is associated with that point. That is at any instant \( t \),

\[
 \epsilon_M(x_M, t) = \frac{1}{|\Omega_m|} \int_{\Omega_m} \epsilon_m(x_m, t) \, d\Omega \quad (2.42)
\]
where \( |\cdot| \) denotes the measure of the domain e.g., the area in two dimensions and the volume in three dimensions.

The above can be elaborated further as follows\(^\dagger\)

\[
\epsilon_M = \frac{1}{|\Omega_m|} \int_{\Omega_m} \frac{1}{2} \left( u^m_{ij} + u^m_{ji} \right) d\Omega \\
= \frac{1}{|\Omega_m|} \int_{\Gamma_m} \frac{1}{2} \left( u^m_i n_j + u^m_j n_i \right) d\Omega = \frac{1}{|\Omega_m|} \int_{\Gamma_m} \mathbf{u}_m \otimes^{\text{sym}} \mathbf{n} d\Gamma
\]  

(2.43)

where the definition of the strain tensor was used in the first equality and the Gauss theorem was adopted to convert a domain integral into a surface integral in the second equality. In the above, \( \mathbf{n} \) denotes the unit outward normal to \( \Gamma_m \), \( \mathbf{u}_m \) denotes the microscopic displacement field and \( \otimes^{\text{sym}} \) denotes the symmetrized dyadic product which is defined as

\[
\mathbf{a} \otimes^{\text{sym}} \mathbf{b} = \frac{1}{2} (\mathbf{a} \otimes \mathbf{b} + \mathbf{b} \otimes \mathbf{a})
\]

(2.44)

Without loss of generality, the microscale displacement field can be additively decomposed as follows \[152\]

\[
\mathbf{u}_m(x_m, t) = \epsilon_M(x_M, t) \cdot x_m + \tilde{\mathbf{u}}_m(x_m, t)
\]

(2.45)

where \( \tilde{\mathbf{u}}_m(x_m, t) \) is the microscale displacement fluctuation field that is added to the linear displacement field \( \epsilon_M(x_M, t) \cdot x_m \) to account for the contribution of heterogeneities.

By substituting Equation (2.45) into Equation (2.43), one obtains

\[
\epsilon_M = \frac{1}{|\Omega_m|} \int_{\Gamma_m} (\epsilon_M \cdot x_m \otimes^{\text{sym}} \mathbf{n} + \tilde{\mathbf{u}}_m \otimes^{\text{sym}} \mathbf{n}) d\Gamma
\\
= \epsilon_M + \frac{1}{|\Omega_m|} \int_{\Gamma_m} \tilde{\mathbf{u}}_m \otimes^{\text{sym}} \mathbf{n} d\Gamma
\]

(2.46)

This means that in order to satisfy the strain averaging theorem given in Equation (2.42), the microscale displacement fluctuation field must fulfill the following

\(^\dagger\)We have switched the position of the subscript \( m \) to superscript when indicial notation was used for convenience of reading.
\[ \int_{\Gamma_m} \mathbf{u}_m \otimes \text{sym} \mathbf{n} \, d\Gamma = 0 \quad (2.47) \]

**Hill-Mandel macro-homogeneity principle**

Based on physical arguments, the Hill-Mandel macro-homogeneity principle \([70, 105]\) establishes that the macroscopic stress power must equal the volume average of the microscopic stress power over the RVE. That is, at any state of the RVE characterized by a stress field \( \sigma_m \) in equilibrium,

\[
\sigma_M : \dot{\epsilon}_M = \frac{1}{|\Omega_m|} \int_{\Omega_m} \sigma_m : \dot{\epsilon}_m \, d\Omega \quad (2.48)
\]

must hold for any \( \dot{\epsilon}_m \). The symbol : indicates the double contraction operator when applied for two second order tensors \( A \) and \( B \) yields \( A : B = A_{ij}B_{ij} \).

The RHS of Equation (2.48) can be elaborated as

\[
\sigma_M : \dot{\epsilon}_M = \frac{1}{|\Omega_m|} \int_{\Gamma_m} \mathbf{t}_m \cdot \mathbf{u}_m \, d\Gamma = \frac{1}{|\Omega_m|} \int_{\Gamma_m} \mathbf{t}_m \cdot (\dot{\epsilon}_M \cdot \mathbf{x}_m + \dot{\mathbf{u}}_m) \, d\Gamma
\]

\[
= \left( \frac{1}{|\Omega_m|} \int_{\Gamma_m} \mathbf{t}_m \otimes \mathbf{x}_m \, d\Gamma \right) : \dot{\epsilon}_M + \frac{1}{|\Omega_m|} \int_{\Gamma_m} \mathbf{t}_m \cdot \dot{\mathbf{u}}_m \, d\Gamma \quad (2.49)
\]

where use was made of the weak form and Equation (2.45) in the first equality. The microscopic traction vector is denoted by \( \mathbf{t}_m \).

If the microscopic displacement fluctuation \( \mathbf{u}_m \) is chosen such that the second term of the RHS of Equation (2.49) is vanished, e.g., the microscopic fluctuation field does not contribute to the microscopic work then we have

\[
\sigma_M(x_M, t) = \frac{1}{|\Omega_m|} \int_{\Gamma_m} \mathbf{t}_m \otimes \mathbf{x}_m \, d\Gamma = \frac{1}{|\Omega_m|} \int_{\Omega_m} \sigma_m(x_m, t) \, d\Omega \quad (2.50)
\]

This indicates that the macroscopic stress tensor is defined as the volume average of the microscopic stress tensor.
Availability of constitutive behaviour of RVE’s constituents

Although the constitutive behaviour of the material at the macroscale is not needed *a priori* in a CH framework, the behaviour of the microstructural constituents must be identified prior to the simulation. This can be achieved with phenomenological constitutive models of which parameters are determined using conventional parameter identification processes e.g., experiments and/or inverse analysis (refer to [77] for instance and references therein) but now applied for individual microstructural constituents. Alternatively, constitutive models for the microscale phases can be defined using a numerical homogenization procedure or even a computational homogenization scheme by going one more scale down.

2.4.3 Computational aspects

**Boundary conditions imposed on the RVE** Basically, there are three types of boundary conditions (BCs) which are employed in computational homogenization namely (i) linear BCs\(^\dagger\) (ii) periodic boundary fluctuations and (iii) constant tractions. Since in [185, 192] authors have proved that even for non-periodic heterogeneous materials, periodic BCs provide reasonable estimates of the effective properties, this boundary condition is chosen in this thesis to predict effective properties for the bulk material.

**Remark 2.4.1.** In literature, some other BCs have been proposed as well. In [119] the authors argue that periodic BCs impose unphysical constraints on the unit cell, for example periodic BCs result in a stiffer constitutive response under shear loading. They propose the use of Minimal Kinematic BCs, in which the macroscopic loading is satisfied in a weak sense through a boundary integral, rather than at every point in the material domain. In [13], a combination of linear BCs and constant traction BCs is used for a cracked unit cell. The latter is used for the boundary in the neighborhood of a crack whereas the former is adopted for the remaining boundary. Note that we presented various BCs used in CH schemes just for completeness.

Considering a periodic RVE shown in Figure 2.13. The opposite edges of the RVE \(\Gamma_{m,i}^+ \) and \(\Gamma_{m,i}^-\) have the same length and \(\mathbf{n}_i^+ = -\mathbf{n}_i^-\). Then, the periodic BCs state that the displacement fluctuation is periodic on the boundary of the RVE whilst the traction is anti-periodic on \(\Gamma_m\). That is

\[ u_m(x_m, t) = \varepsilon_M(x_M, t) \cdot x_m. \]

\(^\dagger\)The microscale displacement is given by \(u_m(x_m, t) = \varepsilon_M(x_M, t) \cdot x_m.\)
Figure 2.13 Periodic representative volume element.

\[ \tilde{u}_m(x^+) = \tilde{u}_m(x^-), \quad t(x^+) = -t(x^-) \] (2.51)

To show that periodic BCs satisfy the strain averaging theorem, Equation (2.47) is equivalently written as

\[ \sum_{i=1}^{\frac{1}{2}} \left( \int_{\Gamma_m^+} \tilde{u}_m \otimes \mathbf{n}_i^+ \, d\Gamma + \int_{\Gamma_m^-} \tilde{u}_m \otimes \mathbf{n}_i^- \, d\Gamma \right) = 0 \] (2.52)

Substitution of the first equation in Equation (2.51) into the above and utilization of the fact that \( \mathbf{n}_i^+ = -\mathbf{n}_i^- \), we find that Equation (2.52) is indeed verified. Furthermore, it can be easily verified that with Equation (2.51), the microscopic displacement fluctuation does not do work on the boundary i.e., \( \int_{\Gamma_m} \mathbf{t} \cdot \delta \tilde{u}_m \, d\Gamma = 0 \).

By combining Equations (2.45-2.51), one obtains

\[ u_{r_m^1} - u_{r_m^-} = u_4 - u_1, \quad u_{r_m^2} - u_{r_m^-} = u_2 - u_1 \] (2.53)

with \( u_q \) (\( q = 1, 2, 4 \)), the displacements of controlling node \( q \) given by

\[ u_q = \mathbf{e}_M \cdot \mathbf{x}_q = H_q^T \mathbf{e}_M, \quad H_q = \frac{1}{2} \begin{bmatrix} 2x & 0 & 0 \\ 0 & 2y & 0 \\ y & x & 0 \end{bmatrix}_q, \quad \mathbf{e}_M = \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{12} \end{bmatrix}_M \] (2.54)
where \((x, y)_q\) denotes the coordinates of node \(q\) with respect to a microscopic coordinate system (e.g., one with origin at node 1). By putting \(u_q\) in one vector \(u_b = \begin{bmatrix} u_1; u_2; u_4 \end{bmatrix}^T\), one can write

\[
\begin{bmatrix} H_1 & H_2 & H_4 \end{bmatrix}^T \mathbf{c}_M
\]

(2.55)

**Remark 2.4.2.** The constraints given in Equation (2.53) are handled using Lagrange multipliers in [120]. Here, we are using the master-slave method [46] to impose these constraints, refer to Chapter 6, Section 6.3.1 for details, of which benefit is the lack of additional unknowns.

**Remark 2.4.3.** The aforementioned treatment of periodic BCs is referred to as a strong format according to [96]. This strong format of periodicity imposes a constraint on the mesh topology of the RVE that cannot be fulfilled when adaptive computations are about to be done on unstructured RVE meshes. A weak format of periodic BCs has been proposed in [96] by which a periodic RVE mesh is no longer required.

**Macroscopic stress** The macroscopic stress tensor that is generally defined by Equation (2.50) is simplified as follows in the case of periodic BCs [86]

\[
\sigma_M = \frac{1}{|\Omega_m|} \int_{\Gamma_m} t_m \otimes x_m d\Gamma = \frac{1}{|\Omega_m|} \sum_{i=1,2,4} f_i \otimes x_i
\]

(2.56)

Written in matrix-vector notation, the macroscopic stress vector reads

\[
\sigma_M = \frac{1}{|\Omega_m|} \begin{bmatrix} H_1 & H_2 & H_4 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_4 \end{bmatrix} = \frac{1}{|\Omega_m|} Hf_b
\]

(2.57)

**Macroscopic tangent moduli** To retain the quadratic convergence property of the Newton-Raphson method used to solve the macroscopic BVP, it is desirable to derive the so-called consistent tangent \(D_M\)

\[
\delta \sigma_M = D_M \delta \mathbf{c}_M
\]

(2.58)

At the converged state, the linear system of equations of the RVE can be written as \(K_{ii} \delta u_{ii} = \delta f_{ii}\) where \(i\) represents independent dofs. This system is partitioned as follows
2.4 Continuous computational homogenization model

\[
\begin{bmatrix}
K_{aa} & K_{ab} \\
K_{ba} & K_{bb}
\end{bmatrix}
\begin{bmatrix}
\delta u_a \\
\delta u_b
\end{bmatrix}
= \begin{bmatrix}
0 \\
\delta f_b
\end{bmatrix} \tag{2.59}
\]

in which \( b \) represents degrees of freedom (dofs) associated with the three controlling nodes 1, 2 and 4. Dofs associated with the remaining nodes (e.g., the independent nodes suppressing the controlling nodes) are denoted by \( a \).

Using the standard static condensation gives the equation which involves only controlling dofs

\[
K_{bb} \delta u_b = \delta f_b, \quad K_{bb} = K_{bb} - K_{ba}K_{aa}^{-1}K_{ab} \tag{2.60}
\]

The variation of the macroscopic stress vector is given by, see Equation (2.57)

\[
\delta \sigma_M = \frac{1}{|\Omega_m|}H\delta f_b = \frac{1}{|\Omega_m|}H \bar{K}_{bb} \delta u_b = \frac{1}{|\Omega_m|}H \bar{K}_{bb} H^T \delta e_M \tag{2.61}
\]

where Equations (2.55) and (2.60) have been used. Comparing this equation with Equation (2.58) gives the following macroscale tangent moduli matrix

\[
D_M = \frac{1}{|\Omega_m|}H \bar{K}_{bb} H^T \tag{2.62}
\]

A naive implementation of CH scheme would involve partition of the microscopic stiffness matrix into sub-matrices, see Equation (2.59) and inversion of them. Apparently this implementation is not efficient for RVE meshes with a large number of elements. In this thesis, we are going to present a new way to compute \( D_M \) without partitioning and inverting any matrix.

**Summary of the continuous CH scheme**

Given a macroscopic strain vector \( e_M \) of an integration point, one is seeking for the corresponding macroscopic stress vector \( \sigma_M \) and the macroscopic material tangent \( D_M \). The procedure, usually referred to as a multiscale constitutive box, is given in Box 1.
Box 1 Procedure of the continuous CH scheme (at level of macroscopic integration points).

1. **Downscaling** or macro-to-micro transition. The macroscopic strain vector $\mathbf{\epsilon}_M$ is transformed to the RVE as boundary conditions, see Equation (2.55). Note that the specific BCs must fulfill the **strain averaging theorem**.

2. The BVP of the RVE (in short, the micro-BVP) is solved.

3. **Upscaling** or micro-to-macro transition. The microscopic stresses are upscaled to the macroscale as the macroscopic stress vector, refer to Equation (2.57). This is achieved based on the **Hill-Mandel principle**. Besides, the microscopic stiffness matrix is upscaled to the macroscopic material tangent, see Equation (2.62).

### 2.4.4 Limitation of continuous CH applied for softening materials

When strain localization occurs at the RVE level, the homogenized constitutive equation $\sigma_M - \mathbf{\epsilon}_M$ is a strain softening constitutive equation. The severe consequence of this is that the macroscopic BVP is ill-posed or in mathematical terms, the macroscopic BVP loses ellipticity. Therefore, the numerical solution obtained with CH theory when softening materials are adopted at the microscale is sensitive with respect to the macroscopic finite element discretization. This has been shown in [59] and recently in [6], the author has questioned the applicability of standard/conventional CH theory for softening materials.

One of the basic assumptions in homogenization theory is the existence of a representative volume element. It means that when using a microscopic sample which is larger than the RVE, the macroscopic response should remain unchanged. As shown in [60], this is the case for non-softening materials but not for softening materials since the material loses statistical homogeneity upon strain localization.

In summary, when applied for softening materials, the continuous/bulk CH theory suffers from two problems namely (i) the macroscopic BVP is ill posed and (ii) the method is not objective with respect to the size of the RVE.

In recent years attempts have been made to overcome the aforementioned drawbacks of continuous CH schemes for softening materials. They
include the second-order CH scheme presented in [87], the discontinuous CH scheme in [108, 115–117] for masonry materials, the coupled-volume method [59] (this method is very similar to the fracture energy model [8]) and most recently the discontinuous CH scheme for crack homogenization [194]. Yet another method is the Multiscale Aggregating Method (MAD) presented in [13, 15].

In this thesis, a new technique, the failure zone averaging scheme, is presented (refer to Chapter 4) by which the aforementioned second drawback of the continuous CH scheme is eliminated. Using this new averaging scheme, discontinuous CH models for softening materials are developed (refer to Chapters 5 and 7) which are insensitive with respect to the macroscopic FE discretization and objective with respect to the size of the microscopic sample.

Remark 2.4.4. The aforementioned continuous CH scheme (see Figure 2.12) is classified as a first-order (i.e., only the first gradient of the macroscopic displacement field is transferred to the microscale) homogenization scheme according to [87] in which the authors have presented a second-order CH method. Refer to [81, 88] and references therein for recent studies on this second-order CH method. Note that second-order CH schemes cannot properly deal with softening materials exhibiting deformation beyond a quadratic nature in the displacements [53].

2.5 Discontinuous computational homogenization models

Discontinuous CH schemes determine constitutive relations for macroscopic solids made of heterogeneous materials that exhibit weak and/or strong discontinuities at the macro and/or micro scales. To the best knowledge of the author, the first discontinuous CH scheme for modeling weak discontinuities in heterogeneous solids is the work given in [108]. In this method (developed for masonry materials), a discontinuity band is embedded in the macroscopic solid when localization is detected at the microscopic sample. The behaviour of the discontinuity band is derived from nested microscopic FE computations. This scheme has been extended in [115] to model strong discontinuities i.e., cracks in masonry materials in which the initially rigid cohesive law of the macroscopic crack is computed from nested microscopic FE computations. In these works, microscopic failure is treated with a damage model. Another discontinuous CH method for modeling cracked heterogeneous solids has been reported in [194]. The
extrinsic cohesive law for the macroscopic crack is defined from nested FE computations realized on a microscopic sample that exhibits discrete cracking.

Homogenization towards intrinsic cohesive laws that govern the behaviour of heterogeneous material layers has been presented in [2, 91, 110]. Computational homogenization for heterogeneous material layers has been given in [73, 92, 194].

In summary, discontinuous CH schemes include (i) the CH model for weak discontinuities [108], (ii) the CH model for cohesive cracks [115, 194], (iii) the CH model for material layers [110] and (iv) the MAD presented in [13, 15]. In this work, we develop discontinuous CH models which are somehow similar to models given in [73, 194]. Therefore, these two methods are briefly discussed in the following.

### 2.5.1 Homogenization towards initially elastic cohesive law

Considering a solid with a heterogeneous material layer, see Figure 2.14. The thickness of the layer is denoted by $t_{adh}$. At the macroscale, the finite thickness layer is modelled as a set of zero thickness interface elements the behavior of which e.g., the initially elastic cohesive law is coming from microscale FE computations performed on a micro-sample with the height being $t_{adh}$, and the microstructure of the layer is fully resolved.

![Figure 2.14](image)

**Figure 2.14** A two-dimensional solid with a heterogeneous layer.

The general procedure of the scheme is given in Figure 2.15a. Boundary conditions applied on the RVE are shown in Figure 2.15b. It is emphasized that these BCs are defined intuitively based on the geometry interpretation of the problem. Periodic BCs on the left and right edges read $u_L = u_R$ and $t_R = -t_L$. 
The micro-to-macro transition is also based on the Hill-Mandel principle that now reads

$$ t_M \cdot \delta [\mathbf{u}]_M = \frac{1}{h} \int_{\Gamma_m} t_m \cdot \delta \mathbf{u}_m d\Gamma_m $$  \hspace{1cm} (2.63)

where $h$ denotes the width of the micro sample. Note that since the material layer is modelled as a line at the macroscale, homogenization of the material layer is one-dimensional homogenization along the direction parallel to the
Chapter 2 Numerical modelling techniques for damage and fracture

The above equation can be rewritten as follows (see Figure 2.15b for notations)

\[ t_M \cdot \delta[u]_M = \frac{1}{h} \left[ \left( \int_{\Gamma_t} t_m d\Gamma_m \right) \cdot \delta[u]_M + \int_{\Gamma_R} t_m (\delta u_R - \delta u_L) d\Gamma \right] = \frac{1}{h} \left( \int_{\Gamma_t} t_m d\Gamma_m \right) \cdot \delta[u]_M \tag{2.64} \]

where periodic BCs of the displacements on the right and left edges together with anti-periodicity of the traction on these edges have been used. Since this equation holds for any \( \delta[u]_M \), one obtains

\[ t_M = \frac{1}{h} \int_{\Gamma_t} t_m d\Gamma_m \tag{2.65} \]

This line of derivation shares similarity with the one given in [2].

As shown in [2, 91, 110], when \( h \) is sufficiently large (note that \( t_{adh} \) is kept fixed), the homogenized initially elastic cohesive law \( (t_M, [u]_M) \) becomes independent of \( h \). In other words, an RVE exists for this kind of homogenization.

### 2.5.2 Homogenization towards initially rigid cohesive law

The discontinuous homogenization scheme for modelling cohesive failure in heterogeneous solids presented in [194] is given in Figure 2.16. The macroscopic bulk is assumed to be linear elastic with effective properties computed a priori using the continuous CH model presented in Section 2.4. When the macroscopic stresses satisfy a failure criterion, a crack is inserted at the macroscale. The extrinsic cohesive law of the crack is computed from nested FE computations realized on micro samples attached to GPs on the crack. Microscale failure is represented by discrete cracks.

The Hill-Mandel theorem for the micro-to-macro transition reads [194]

\[ \sigma_M : \delta e_M + \frac{1}{w} t_M : \delta[u]_M = \frac{1}{wh} \int_{\Gamma_m} t_m \cdot \delta u_m d\Gamma \tag{2.66} \]

We are going to prove that the above equation is equivalent to the following Hill-Mandel equation which indicates that the behaviour of the macro crack is coming from the micro cracks.
\[ \dot{\sigma}_M = D \dot{e}_M \]
\[ \tau_M = T_M \overline{[\mathbf{u}]}_M \]

**Figure 2.16** Discontinuous CH scheme for cohesive crack modelling in heterogeneous solids where microscopic failure is represented by discrete cracks.

\[ \mathbf{t}_M \cdot \delta[\mathbf{u}]_M = \frac{1}{h} \int_{\Gamma^c_m} \mathbf{t}_m \cdot \delta[\mathbf{u}]_m d\Gamma \quad (2.67) \]

The proof is as follows. The microscale virtual work equation reads

\[ \int_{\Omega_m} \mathbf{\sigma}_m : \delta \mathbf{e}_m d\Omega + \int_{\Gamma_m} \mathbf{t}_m \cdot \delta[\mathbf{u}]_m d\Gamma = \int_{\Gamma_m} \mathbf{t}_m \cdot \delta \mathbf{u}_m d\Gamma \quad (2.68) \]

where the first part representing the internal work done by the bulk material and the second part expressing the internal work performed by the micro cracks and the third part denoting the external work.

The Hill-Mandel condition for the bulk reads

\[ \mathbf{\sigma}_M : \delta \mathbf{e}_M = \frac{1}{wh} \int_{\Omega_m} \mathbf{\sigma}_m : \delta \mathbf{e}_m d\Omega \quad (2.69) \]

Substitution of Equations (2.67) and (2.69) into Equation (2.68) yields Equation (2.66). This concludes the proof.

It has been shown, in [194], when there is a dominant crack running through the microscopic sample, the homogenized cohesive law is objective with respect to the size of the microscopic sample. Note that Equation (2.67) ensures the objectivity of the homogenized cohesive law.
Chapter 3

Micromechanical modelling of concrete*

In this chapter, we present results of the mechanical behavior of hardening cement paste (CP). The cement paste, at micro level, is composed of unhydrated cement particles, hydration products and capillary pores. It is the topology of this microstructure of the CP that controls the behaviour of concrete at mesoscale and macroscale. We have used a cement hydration model described in [19, 129, 174] to create the microstructure of the cement paste. This microstructure is then discretized into finite elements upon which a simple nonlocal damage constitutive law is applied to each microstructural constituent. The microscale result will be used in a mesoscale model thereby forming a micro-meso two-scale damage model for concrete to be presented in Chapter 8. Since our work employs purely computational techniques, it complements experimental mechanics particularly at the microscale, because it is difficult or even impossible to perform experiments on concrete samples at this very small scale (typically about 100 µm). The analysis presented in this chapter focusses on the microscale of concrete specimens.

The employed procedure is such that a three-dimensional (3D) representation of the CP is obtained through cement hydration simulations of which a slice is input to a mesh generation code that produces a mesh which will be used for two-dimensional (2D) mechanical tests, see Figure 3.1.

The remainder of the chapter is organized as follows. The utilized cement hydration model is described in Section 3.1. The next section presents the finite element model whereas Section 3.3 gives some numerical examples.

3.1 Numerical cement hydration model

To simulate the microstructure of cement paste, we have used the cement hydration model of [129] and implemented it in a flexible object-oriented C++ framework following the work described in [19]. For details on the theory of cement hydration and microstructural development, refer to, among

* Based on references [134, 140]
Figure 3.1 Procedure of numerical modelling of cement pastes: (a) unhydrated cement paste, (b) 3D microstructure after hydration, (c) a 2D section and (d) FE mechanical analysis (the contour plot shows the localization band by means of a damage profile).

others, [17, 18, 190] and references therein. It is emphasized that the cement particles are modelled as spheres of arbitrary size. Moreover, if a sufficiently large number of particles, say one million particles, is adopted the assumption on spherical shape for the particles is good enough to model a realistic microstructure of CP. Although the implemented model is, in principle, able to model any particulate chemical reaction, in this dissertation only the reaction of tricalcium silicate (C₃S) with water producing silicate hydrates (CSH) and Portlandite (CH) is considered.

3.1.1 Initial particle distribution

The water to cement ratio \( w_c \) is defined as the ratio of the water mass to the mass of cement and therefore given by
3.1 Numerical cement hydration model

\[ w_c = \frac{1 - f}{\rho_c f} \]  

(3.1)

where \( f \) is the initial volume fraction of cement, \( \rho_c \) is the density of cement (3.15 g/cm\(^3\)) and we have assumed that the water density is 1.0 g/cm\(^3\).

The total number of cement particles together with their radii can be determined from (i) the water to cement ratio \( w_c \), (ii) the particle size distribution (PSD) of which an example is given in Table 3.1 where each value in the second column denotes the volume fraction of powder whose size is smaller than the value given in the first column and (iii) the computational volume which is usually a cube, say 100 × 100 × 100 µm\(^3\). These particles are then randomly placed into the volume without overlapping, see for instance Figure 3.1a. A more realistic way is to firstly perform a particle packing simulation to obtain a particle distribution that is able to simulate natural phenomena such as clustering, size segregation. In this case considerably higher densities can be reached. The cement hydration simulation starts with this dense particle distribution [175].

<table>
<thead>
<tr>
<th>( d ) [µm]</th>
<th>( f ) [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.71</td>
<td>0.000</td>
</tr>
<tr>
<td>6.84</td>
<td>0.301</td>
</tr>
<tr>
<td>9.05</td>
<td>0.396</td>
</tr>
<tr>
<td>21.0</td>
<td>0.738</td>
</tr>
<tr>
<td>30.5</td>
<td>1.000</td>
</tr>
</tbody>
</table>

Table 3.1 A typical cumulative volume distribution.

3.1.2 Chemical reactions

When cement contacts with water, numerous complex chemical reactions take place. However, here, we focus only on the reaction of the tricalcium silicate \( \text{C}_3\text{S} \) that is the most important component of cement. Since we are interested in modelling the microstructure, the reaction is written in terms of volume rather than mass as follows

\[ 1.0V_{\text{C}_3\text{S}} + 1.318V_{\text{H}_2\text{O}} \rightarrow 1.57V_{\text{CSH}} + 0.593V_{\text{CH}} \]  

(3.2)
where $V_a$ denotes the volume of phase $a$.

### 3.1.3 Reaction kinetics

In this dissertation, we have employed the standard reaction kinetics, namely nucleation and growth, phase boundary and diffusion which are expressed mathematically by the following equations, respectively [190]

\[
\begin{align*}
    dr_{in} &= -nk_1t^{n-1} \exp^{-k_1t^n} dt \\
    dr_{in} &= -k_2 dt \\
    dr_{in} &= -\frac{k_3}{r_{out} - r_{in}} dt
\end{align*}
\]  

(3.3a)  (3.3b)  (3.3c)

where $dr_{in}$ represents the change in radius due to the reaction of the cement, $t$ refers to the hydration time; $n$, $k_1$, $k_2$ and $k_3$ denote the kinetics constants. The inner radius and outermost radius of a hydrating particle are represented by $r_{int}$ and $r_{out}$ respectively, see Figure 3.2.

At any time step, the kinetics differ from particle to particle and the equation that gives the slowest rate in the three aforementioned kinetic equations is chosen. Since interaction between hydrating particles decreases the free surface for water to contact with the particles, the hydration kinetics is modified in order to take this into account as follows [129]

\[
    dr_{int} = dr_{int}^o S_{free} \beta
\]  

(3.4)

where $dr_{int}^o$ is the radius change before taking into account reduction due to a limited free surface (it is computed according to Equation (3.3)) and $S_{free}$ denotes the free surface area of the cement particle. The parameter $\beta$ accounts for other factors such as water consumption, curing temperature or chemical composition. In the current implementation, only the former is considered using a correction factor given in [190]

\[
    dr_{int} = dr_{int}^o S_{free} \left( 1 - \frac{\alpha v}{\rho w_o + \alpha} \right)
\]  

(3.5)

where $\alpha$ is the degree of hydration, $v$ is the ratio between the volume of the reaction products and the volume of the reactant, $w_o$ is the initial water to
cement ratio, \( \rho \) denotes the ratio between the specific mass of C\(_3\)S and the specific mass of water.

The degree of hydration \( \alpha(t) \) is defined by

\[
\alpha(t) = 1 - \frac{V_{\text{reactant}}(t)}{V_{\text{reactant}}(t = 0)}
\]

where \( V_{\text{reactant}}(t) \) and \( V_{\text{reactant}}(t = 0) \) are the volumes of the reactants at time \( t \) and time \( t = 0 \), respectively. The degree of hydration varies between zero (for unhydrated CP) and one (for fully hydrated CP).

### 3.1.4 Spatial distribution of the product

The CSH product that results from the reaction, see Equation (3.2), precipitates on the particle, partially filling the space of the reacted C\(_3\)S (inner product) since the total volume of CSH is larger than the reacted C\(_3\)S. The CH products are randomly spaced in the pores [174].

The number of CH particles nucleated in the pore space at a time \( t \) is given by [190]

\[
n_{\text{CH}} = n_{\text{max}}(1 - e^{-bt})
\]

where \( n_{\text{max}} \) is the maximum number of CH grains at complete hydration and \( b \) is a constant. These two parameters are calculated from the work given in [80] in which it was reported that, at complete hydration, there is one CH grain for every five C\(_3\)S grains (approximately, \( n_{\text{max}} \) is equal to one fifth of the number of C\(_3\)S grains) and after one day of hydration, there is one CH grain for every 12.5 C\(_3\)S grains, hence \( b = 0.213 \). The amount of CH
product produced is then either randomly distributed to these \( n_{CH} \) particles or based on the available surface of the CH particles.

In Figure 3.3 the microstructure of a hardening CP saved as images are given in which two-dimensional (2D) images are used to generate finite element meshes on which mechanical simulations can be performed. Another feature of the program is the capacity to visualize the microstructure of the pores, see Figure 3.4.

### 3.2 Finite element model

This section describes the finite element model utilized to analyze the mechanical response of a hardening CP. First, the spatial discretization of a CP sample into finite elements is presented. Second, the constitutive behaviour and the material parameters of different phases of a CP are provided. Finally, the influence of the pores on the response of a CP sample is discussed.

#### 3.2.1 Finite element discretization

A common issue in micromechanical finite element computations is the discretization of microstructures that are typically complex multi-phase materials. The obvious solution is to utilize a compatible mesh, see Figure 3.5a. In case that structured meshes are preferable, say when combined with multi-grid solvers, the Gauss point method proposed by [204] (see Figure 3.5b) or the hanging node method developed in [103] (see Figure 3.5c) might be suitable alternatives to the compatible meshes. XFEM in combination with the level set method (LS) (see Figure 3.5d) have also been adopted to model microstructure independently of the mesh, see among others [97, 125, 180]. An advanced meshing code is presented in [43] that is able to generate both 2D and 3D compatible meshes of a hardening cement paste.

When dealing with complicated 3D microstructure of cement pastes, none of the Gauss point method, the hanging node method and XFEM/LS is applicable, at least practically. This can be explained by the fact that utilizing those methods leads to non-standard finite element formulations that unnecessarily complicate the problem. This might explain the reason in [68] why the 3D CP specimen is meshed by replacing each voxel by one eight-node hexahedron element. Although this meshing technique is simple, it creates, however, meshes containing too many elements which necessitates the use of parallel computing.
Figure 3.3 Different kinds of image output generated by the cement hydration program.

3D microstructure

2D slice with depth perception

2D slice
Since meshing the whole 3D CP specimen will result in a too large FE problem, we had to confine to two-dimensional FE computations on slices of a 3D cement paste. To mesh the microstructure of the cement paste we have used the meshing module of the OOF program [28]. The input of OOF’s mesher is a digital image which can easily be obtained from the cement hydration program. Figure 3.6 shows an example of using OOF’s mesher to obtain the unstructured compatible mesh of a slice of three-dimensional CP.

![Microstructure of the pores as generated by the cement hydration program.](image)

**Figure 3.4** Microstructure of the pores as generated by the cement hydration program.

![Different meshing strategies for multi-phase materials: (a) Compatible mesh, (b) Gauss point method, (c) Hanging node method and (d) XFEM/LS method (black squares denote enriched nodes).](image)

**Figure 3.5** Different meshing strategies for multi-phase materials: (a) Compatible mesh, (b) Gauss point method, (c) Hanging node method and (d) XFEM/LS method (black squares denote enriched nodes).

The meshing procedure is as follows. Starting from an image of a slice, the materials are assigned to different phases based on the color, or more precisely the gray scales of different phases of the image. The meshing process starts with a regular triangle/quadrilateral mesh superimposed on the
3.2 Finite element model

Figure 3.6 Meshing the microstructure of cement paste using the OOF program.

whole image. This regular mesh is then refined adaptively by minimizing a cost function which is the sum of energy value $E$ of all elements. The element’s energy $E$ is defined as a linear combination of a shape parameter $E_{\text{shape}}$ and a homogeneity parameter $E_{\text{hom}}$:

$$E = \theta E_{\text{hom}} + (1 - \theta) E_{\text{shape}}; \quad 0 \leq \theta \leq 1$$  \hspace{1cm} (3.8)

where $\theta$ is a weighting factor that controls the relative importance of element shape and homogeneity; $\alpha = 0$ emphasizes shape and ignores homogeneity while $\alpha = 1$ emphasizes homogeneity and ignores shape.

The shape parameter $E_{\text{shape}}$ indicates to which extent much a triangle element differs from being an equilateral, and is given by
where \( A \) and \( L \) are the area and perimeter of a triangle element, respectively.

The homogeneity parameter \( E_{\text{hom}} \) measures the homogeneity of the element. It is minimized with a value of zero when the element contains only one material. It is defined as

\[
E_{\text{hom}} = \prod_i \frac{1 - a_i(T)}{1 - \frac{1}{N}}
\]  

(3.10)

where \( N \) denotes the number of pixel categories i.e., the number of micro-phases and \( a_i(T) \) represents the area fraction of phase \( i \) in element \( T \). These two parameters can be easily understood by the illustration given in Figure 3.7.

![Figure 3.7](image)

**Figure 3.7** Shape (a) and homogeneity (b) parameters used in adaptive meshing, taken from [28].

### 3.2.2 Constitutive models

In order to simulate the tensile damage of the CP, we have employed the simple isotropic damage model regularized by the gradient enhanced method, refer to Chapter 2, Section 2.2.1. The values of the various material parameters are given in Table 3.2. The Young’s moduli and Poisson ratios, which are normally obtained through nano-indentation methods, are taken from [31, 68] whereas the inelastic parameters have been chosen without experimental reference since at the time of this writing no experimental data was available. Note that in [68] an inverse analysis was utilized to determine the inelastic parameters. This is however not done here since our target is to propose a fully numerical framework for performing micromechanical
analysis for concrete rather than an extended comparison with experimental results. It should be emphasized that the $c$ parameter is currently not available, the given value was chosen in such a way that there are about three finite elements in the localization band. However, $c$ should be linked to the microstructural properties such as the cement particle size for instance and the FE mesh should be fine enough to resolve the localization bandwidth coupled to this $c$ value.

<table>
<thead>
<tr>
<th></th>
<th>Unhydrated</th>
<th>Hydrates</th>
<th>Pore</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [N/mm$^2$]</td>
<td>132 700</td>
<td>24 000</td>
<td>1.0</td>
</tr>
<tr>
<td>$\nu$ [-]</td>
<td>0.3</td>
<td>0.24</td>
<td>0.0</td>
</tr>
<tr>
<td>$\kappa_I$ [-]</td>
<td>-</td>
<td>5e-06</td>
<td>-</td>
</tr>
<tr>
<td>$\gamma$ [-]</td>
<td>-</td>
<td>0.95</td>
<td>-</td>
</tr>
<tr>
<td>$\beta$ [-]</td>
<td>-</td>
<td>1500</td>
<td>-</td>
</tr>
<tr>
<td>$c$ [mm$^2$]</td>
<td>-</td>
<td>8e-6</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 3.2 Material parameters of different phases of a hardening cement paste.

Remark 3.2.1. It can be seen from Tab. 3.2 that, for unhydrating particles and pores (in case the pore space is meshed), no value was assigned for the inelastic parameters $\kappa_I, \gamma, \beta$ and $c$. In other words, an elastic model was used for these phases while the gradient enhanced damage model was utilized for the hydrates. Therefore, there is no nonlocal interaction between different phases.

3.2.3 Pore modelling

In [68], Section 4.2.1 page 203, the authors stated that “a stable finite element calculation must include pores since preliminarily removing unconnected voxels is computationally costly”. They have chosen, based on a series of numerical computations in the linear elastic regime, the values of the Young’s modulus and the Poisson ratio for the pores to be of unity and zero, respectively. Here we are interested in the effect of modelling the pores in the post peak regime. To this end, we are going to compare the response of the cement paste with and without pores being modelled. A simple algorithm to remove unconnected elements is introduced.

To mesh the microstructure without considering the pores, we proceed as follows: (i) meshing the microstructure using OOF as before, however, the
Box 2 Isolated elements removal.

1. Two element sets: accepted (A) and front (F)
2. Choose one element as seed element, put it in A and F
3. while F is not empty, do
   a) pop the first element E of F
   b) get neighbors of E, loop on the neighbors I
   c) if I is not in A, put I in A and F

Neighbors = element sharing one common edge.

pore elements are marked with a special tag; (ii) those elements having this special tag are omitted from the mesh; (iii) the algorithm given in Box 2, a simple application of the fast marching method [161], is then applied to this mesh in order to remove any isolated elements (without doing so, the resulting FE linear system would be singular).

3.3 Numerical results

This section presents an analysis of a hardening CP sample subject to a uniaxial tensile loading. Through the discussion, various issues such as (i) cement hydration simulation (ii) microstructure discretization and (iii) pore modelling will be illustrated.

3.3.1 Cement hydration simulation

The data of the cement hydration simulation is given as follows

- A computational volume of $200 \times 200 \times 200 \, \mu m^3$,
- A water to cement ratio $w_c$ of 0.4,
- Particle diameters range from 0.5 µm to 40 µm according to the sieve curve shown in Figure 3.8 (886 383 cement particles),
- Kinetics constants, see Equation (3.3), $k_1 = 1.14 \times 10^{-4} \, h^{-3}$, $k_2 = 1.0 \, \mu m \, h^{-1}$, $k_3 = 0.01 \, \mu m^2 \, h^{-1}$, $n = 3$ [18].
• Hydration time is eight years.

The computer time for this simulation was about 36 minutes on a laptop (2GB of RAM and speed 2.20 GHz). Figure 3.9 shows the microstructure of the hardening CP at 28 days of hydration. The evolution of the microstructure is given in Figure 3.10.

Figure 3.8 Cumulative volume size distribution of the utilized cement.

Figure 3.9 Microstructure of the hardening CP at 28 days of hydration and the concept of taking two-dimensional slices.
3.3.2 Meshing the microstructure

When the hydration simulation has been finished, images of three slices (along $X$, $Y$ and $Z$ directions) of the CP at a particular hydration time are put into the OOF program to create the corresponding FE meshes. Figure 3.11 shows the FE meshes of the $Z$ slice through the center of the specimen. The red color denotes unhydrated material, the blue color is used for the hydration products and the yellow color represents the pores. The FE meshes consist of approximately 41 000 three-noded triangular elements with the number of degrees of freedom about 61 000. Having the FE meshes, the final step is to carry out damage simulations on these meshes as presented in the following.

3.3.3 Mechanical simulations

We have performed uniaxial tension tests on two meshes, one with the pores of which the elastic parameters are the ones given in Table 5.1 and another one where the pores are not meshed. Figure 3.12 confirms the conclusion given in [68] that in the linear elastic regime, if the pore is modelled its elastic constants should be $E = 1 \text{ N/mm}^2$ and $\nu = 0$. However, in the softening regime, there is a substantial difference between modelling the pore (with $E = 1 \text{ N/mm}^2$ and $\nu = 0$) and not modelling the pore. In order to determine the proper values for the elastic constants of the pore in case it is modelled, the uniaxial tension test previously presented has been conducted again with varying Young’s moduli from 0.001 N/mm$^2$ to 1 N/mm$^2$. Figure 3.13 indicates that the Young’s modulus of the pore must be chosen equal to
3.3 Numerical results

Figure 3.11  FE discretizations of a slice of a CP specimen: with (left) and without (right) meshing pores. The bottom row gives a close-up view of the meshes given in the top row. Note that isolated elements were also removed.

0.001 N/mm². The localized damage distribution in the uniaxially loaded CP is depicted in Figure 3.14.

Finally, the above test is carried out for the cement paste that was hydrated for 28 days, 243 days and 730 days. In Figure 3.15, the result of a uniaxial tension test is shown where $\alpha$ and $f_p$ are the degree of hydration and the pore fraction, respectively. By reducing the Young’s modulus of the pores, the load-displacement curves converge to the one obtained without meshing the pores. For specimens which are more hydrated, see Figure 3.15b-c, even a small reduction in Young’s modulus led to the response obtained without meshing the pores. This is expected since more hydrated material corresponds to less pores.
Figure 3.12  Meshing and no meshing of the pores (at 28 days of hydration): load-displacement comparison for different slices.
3.4 Concluding remarks

In this chapter, a numerical framework for damage analysis of concrete specimens at microscale has been presented. The proposed model, which is a combination of a discrete model (a cement hydration model) and a continuum model (nonlocal damage model) provides a promising means to understand the behaviour of concrete at microscopic scale. Furthermore, it might complement experimental work. The discretization of the microstructure of the cement paste and the effect of meshing the pores in contrast to not incorporating them at all in the mesh have been given. The numerical tests showed that the pores should not be discretized. If the pore space is dis-
Chapter 3 Micromechanical modelling of concrete

cretized, the Young’s modulus of the pores must be chosen carefully. The presented micromechanical model will be utilized in a multiscale model for concrete materials in Chapter 8.
Chapter 4

On the existence of representative volumes for softening materials

A concept of crucial importance of homogenization-based multiscale models is the representative volume element (RVE). There is not a single and exact definition of the RVE for an arbitrary heterogeneous material. That might explain the existence of various definitions of the RVE, see [60] for a recent review. Briefly speaking a microscopic sample is considered to be an RVE when (i) an increase in its size does not lead to considerable differences in the homogenized properties, and (ii) the microscopic sample is large enough so that the homogenized properties are independent of the microstructural randomness. The issue of existence of the RVE for materials that exhibit strain localization (e.g., concrete, soil), however, has been addressed by only a few researchers [58, 60, 61]. It has been shown in [60] that for softening materials an RVE cannot be found using conventional averaging techniques.

However, very recently, in [194] the authors have proved the existence of an RVE for softening materials by deriving a traction-separation law (for a macro crack) from the microscopic stresses and strains instead of a stress-strain relation as is usually done in standard CH schemes. Motivated by the work in [194] this chapter presents a numerical demonstration of the existence of an RVE for a class of softening materials with a random microstructure that exhibits damage in an averaged, smeared fashion. This is in contrast to the material utilized in [194] which shows discrete cracking within a regular microstructure. It is emphasized that the RVE’s existence proof is an important step in the process of developing a homogenization scheme for softening materials with a microstructural length scale that is very small compared to the macroscopic one. In this way, the separation-of-scales principle still applies. Such a scheme will be presented in the next chapter.

In this chapter we develop an adequate averaging strategy that revises

* Based on reference [136]
the existence of the RVE for softening materials. The idea is to average the stresses and strains in the micro samples over a propagating damaged zone rather than over the entire micro sample which is usually the case in standard averaging techniques.

The structure of the remainder of the chapter is as follows. In Section 4.1, the problem statement is given with details concerning the generation of the samples, the utilized constitutive model and the boundary conditions. Section 4.2 presents the proposed averaging scheme followed by a statistical analysis.

4.1 Problem statement

4.1.1 Sample generation

In this thesis, the random heterogeneous material that we investigate is a three-phase material with matrix, aggregates (of circular shape) and an interfacial transition zone (ITZ) surrounding each aggregate. This three-phase material is the so-called mesoscale model for concrete, see for instance [201]. The material samples have been generated using SPACE [176], a discrete element program, with input including the sample size, the size distribution of the aggregates and the density \( \rho \) (volume fraction) of aggregates. Details on the generation procedure can be found in [177]. These samples are then discretized into finite element meshes (three-noded triangular elements). Figure 4.1 shows an example where three phases can be distinguished in the close-up view.

![Figure 4.1](image)

Figure 4.1 Finite element mesh of the three-phase material sample: full view (left) and close-up view (right).

In order to study the effect of the size of the samples on the response of the material, for three aggregate densities \( \rho \) (30%, 45% and 60%), five different sizes varying from \( 10 \times 10 \text{ mm}^2 \) to \( 30 \times 30 \text{ mm}^2 \) as depicted in Figure 4.2 are
4.1 Problem statement

studied. Sizes of aggregates are varied from 2.5 mm to 5.0 mm with a uniformly random distribution. The width of the ITZ is taken 0.25 mm i.e., 10% of the smallest diameter of the aggregates. The randomness of the aggregate distribution is studied by considering four realizations of each sample size, see Figure 4.3. It should be emphasized that four is a small number for a statistical analysis. However it was not the intention of the author to perform a full statistical analysis, instead a statistical study is given to support the result. The three aggregate densities are shown in Figure 4.4.

![Samples of varying sizes for the case of 30% aggregate.](image)

4.1.2 Constitutive model

Failure of the material is modelled using the gradient enhanced damage model presented in Chapter 2, Section 2.2.1. In summary, the utilized constitutive model is fully characterized by six material parameters: the Young’s
modulus $E$, the Poisson’s ratio $\nu$, the three inelastic parameters $\gamma$, $\beta$, $\kappa_I$ and the length scale $c$. These material parameters are tabulated in Table 4.1 along with the values taken for the various constituents. Note that $\kappa_I$ has been set large for the aggregates to prevent damage and the $c$ parameter has been assumed to be the same for all constituents. The material constants are chosen such that the material consists of hard elastic aggregates embedded in a soft damageable matrix with the ITZ as the weakest region. This could be representative for concrete at mesoscale.

<table>
<thead>
<tr>
<th></th>
<th>Matrix</th>
<th>Aggregate</th>
<th>ITZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>[N/mm$^2$]</td>
<td>25 000</td>
<td>30 000</td>
</tr>
<tr>
<td>$\nu$</td>
<td>[-]</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$\kappa_I$</td>
<td>[-]</td>
<td>5e-06</td>
<td>0.5</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>[-]</td>
<td>0.9</td>
<td>0.9</td>
</tr>
<tr>
<td>$\beta$</td>
<td>[-]</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>$c$</td>
<td>mm$^2$</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Table 4.1 Material parameters of different phases.
Remark 4.1.1. In the utilized gradient enhanced damage model, the averaging equation, $\bar{\varepsilon}_{eq} - c \nabla^2 \bar{\varepsilon}_{eq} = \varepsilon_{eq}$, was applied with vanishing normal gradient of the nonlocal equivalent strain as a boundary condition imposed on the external boundary only (see Equation (2.18)). Consequently there are non-local interactions between points belonging to different phases. However this issue is not critical in the present work since the aggregates are elastic and the non-local interactions between the matrix and the ITZ relate to almost similar materials. Interested readers are referred to [89] for related work. We do believe that the conclusions from this chapter would also apply if the issue of non-locality across material interfaces had been taken into account.

Remark 4.1.2. The adopted non-local damage model introduces an additional material parameter, the so-called internal length scale $\sqrt{c}$. This parameter is supposed to represent phenomena occurring at a lower scale. Considering the heterogeneity nature of the matrix (cement paste) at the microscale (unhydrated cement particles, hydration products and pores), it is reasonable to link $\sqrt{c}$ to the microstructure of the matrix. However this link is yet unknown and therefore the value for $c$ as given in Table 5.1 has been chosen without consideration of the microstructure of the matrix. Other material constants such as $E$, $\nu$, $\kappa$, $\gamma$ and $\beta$ can, however, be identified from proper experiments [99, 201].

The failure process of the material obtained with the continuum damage model used in this work is given in Figure 4.5. Going from the top left figure to the down right one, it starts with damage initiation in the ITZ, then the bulk matrix starts to damage. In later stages, damage zones coalesce to eventually form a localization band.

4.1.3 Boundary conditions

An important aspect in RVE-based homogenization methods is the choice of boundary conditions (BCs), which are imposed on the RVE’s boundary, used to capture the effect of the surrounding medium. Commonly used BCs include (i) linear displacements, (ii) uniform traction and (iii) periodic BCs, see Chapter 2, Section 2.4.3 and refer to [120] for a computational treatment of all three BCs. The choice of BCs affects the result of homogenization methods including homogenized properties i.e., macroscale constitutive response, the required size of the RVE and the type (and extent) of localized failure taking place at the microscale. Since linear displacement BCs inhibit
Chapter 4 On the existence of representative volumes for softening materials

Figure 4.5 Failure process occurring in a sample subjected to a uniaxially tensile loading in the horizontal direction.

Localization to occur at the RVE’s boundary (because it maps a straight line in an undeformed RVE to a straight line under deformation), see Figure 4.6, it should not be used for softening RVEs. Uniform traction BCs are also left out of consideration because of the standard strain-driven FE procedure pursued in this work. The issue of choosing proper BCs for damaging RVEs has been discussed in [15, 79].

Figure 4.6 A softening unit cell in shear: linear BCs prevent damage from occurring at the RVE boundary (right) while periodic BCs allows this (left).

In this chapter we utilize, unless otherwise stated, the standard BCs as shown in Figure 4.7 for a uniaxial tension test. Note that this boundary condition has been used in [177] for a study concerning the RVE’s size determination. Furthermore, the main content of this chapter is not about the proper choice of BCs in RVE-based modelling but merely about proving the existence of an RVE for softening materials. Concerning the damage pattern, the difference between the standard BCs and the periodic BCs is that, with
4.1 Problem statement

Figure 4.7 Boundary conditions: utilized (left) and periodic boundary conditions (right).

Figure 4.8 Damage patterns obtained with non-periodic BC and periodic BC.

periodic BCs, the localization band is forced to be periodic as illustrated by Figure 4.8.

In all presented computations a plane strain condition has been used. It should be emphasized that under plane strain condition, the circular aggregates represent long cylinders rather than spherical particles. Therefore the goal was not to formulate a model which would be rigorously representative of concrete.
4.2 Representative volumes and averaging techniques

In literature several definitions for the RVE have been proposed for different materials and purposes, refer to [60] for a recent review. For a specific material, the RVE depends on the physical quantity that is measured. Herein we focus our attention on the mechanical response of a material expressed in terms of the averaged stress and strain evolution.

From various existing definitions of the RVE we consider, in the present context of random heterogeneous materials, a microscopic sample to be an RVE when it fulfills all the following requirements

- an increase in its size (of the same structural realization) does not lead to considerable differences in the homogenized properties
- the microscopic sample is large enough so that the homogenized properties are independent of the microstructural randomness, $l_m \gg d$ see Figure 4.9
- its size is much smaller than the characteristic length $l_M$ over which the macroscopic loading varies in space, $l_m \ll l_M$. This condition is known as the principle of separation of scales.

As has been shown in [60], for quasi-brittle materials, an RVE does exist for the linear and hardening regimes. In the softening regime, however,
[60] questioned the existence of the RVE. In this chapter, a closer look at the problem of RVE’s existence in the softening regime is taken and we will demonstrate that an RVE does exist in the post-peak regime for softening materials. It should be emphasized that in this case the term RVE means RVE for a localization band (or a crack). Figure 4.10 gives a graphical illustration for this revised definition of RVE. Note that in this revised definition of the RVE, the principle of separation of scales states that \( l_m \) should be small enough so that the homogenized quantities are constant over it, we refer to Chapter 6, Section 6.2.1 for more details.

**Figure 4.10** Definition of an RVE for a macroscopic localization zone (thick line). Note that the RVE does not represent (as in its classical meaning) the whole material. It represents for the material on the localization zone.

### 4.2.1 Standard averaging

The homogenized stresses and strains are defined as the volume averages of its microscopic counterparts, see Chapter 2, Section 2.4

\[
\begin{align*}
\langle \sigma \rangle & \equiv \frac{1}{|\Omega_m|} \int_{\Omega_m} \sigma_m d\Omega = \frac{1}{|\Omega_m|} \int_{\Gamma_m} t_i^m x_j^m \mathrm{d}\Gamma \\
\langle \epsilon \rangle & \equiv \frac{1}{|\Omega_m|} \int_{\Omega_m} \epsilon_m d\Omega = \frac{1}{2|\Omega_m|} \int_{\Gamma_m} (u_i^m n_j^m + u_j^m n_i^m) \mathrm{d}\Gamma
\end{align*}
\]

(4.1)

where \( \Omega_m \) denotes the RVE domain (having volume being \(|\Omega_m|\)) with the boundary \( \Gamma_m \); \( \sigma_m \) and \( \epsilon_m \) are the micro stress and strain tensors, respec-
tively; \( t_m \) represents the micro traction vector while \( x_m \) is the position vector and the unit outward normal to \( \Gamma_m \) is given by \( n_m \).

For the considered boundary conditions, refer to Figure 4.7, the homogenized stress and strain along the horizontal direction given in Equation (4.1) are simplified to

\[
\begin{align*}
\langle \sigma \rangle_{xx} &= \frac{f^{\text{int}}_{R,x}}{h}, \\
\langle \epsilon \rangle_{xx} &= \frac{\bar{u}}{w}
\end{align*}
\]  

(4.2)

where \( f^{\text{int}}_{R,x} \) is the sum of all nodal internal forces (x component) along the right edge of the RVE on which an imposed displacement \( \bar{u} \) has been applied in the x-direction, see Figure 4.7.

A plot of the homogenized normal stress-strain diagrams is given in Figure 4.11 for various samples with 30% aggregates. It is obvious that samples of different sizes behave like different materials e.g., the larger the sample the more brittle it is on average. It is based on this kind of behavior plus some additional statistical analysis that [60] questioned the existence of the RVE for softening materials. Although the material model is regularized the response is size dependent. This is caused by the fact that the localization zone does not scale with the size of the RVE, see Figure 4.12.

![Figure 4.11](image)

**Figure 4.11** Response of various concrete samples with 30% aggregate using the standard averaging: the larger the sample the more brittle it is on average—an RVE does not exist for softening materials.

#### 4.2.2 Failure zone averaging

The dependency of the homogenized stress-strain diagrams on the RVE size as discussed in the previous section indicates that standard continuum models cannot be adopted at the macroscale in a homogenization-based
multiscale framework for softening materials. This observation has called for, over the past few years, the development of the so-called coupled volume methods (see for example [59] and references therein), the second-order computational homogenization method [87] and coarse graining of failure methods [13, 15, 108, 115, 194]. The salient feature of coarse graining of failure methods is the introduction of discrete cracks at the macroscale model. We are particularly interested in [194] in which the existence of an RVE for materials undergoing discrete cracking has been demonstrated. The existence of an RVE was indicated by the uniqueness (regardless of the utilized micro sample size) of a macro traction-separation law which has been obtained by averaging the responses along propagating discrete micro cracks.

Prompted by the work given in [194] and the fact that the localization band does not scale with the micro sample size (as can be seen in Figure 4.12), we will present an averaging technique by which homogenized stress-strain relationships are obtained which are objective with respect to the micro sample size.

Let us first denote $\Omega_d$ as the active damaged domain i.e., the region containing Gauss points which are damaged and loading. According to the continuum damage model that we are utilizing herein this domain corresponds to Gauss points satisfying $\omega > 0$ and $f = 0$, mathematically $\Omega_d$ is defined as

$$\Omega_d = \{ x \in \Omega_m | \omega(x) > 0, f(x) = 0 \}$$

(4.3)
refer to Figure 4.13 for a graphical illustration. The active damaged domain is computed as the accumulated tributed area of all Gauss points that are damaged and loading.

**Figure 4.13** Schematic representation of the active damaged domain $\Omega_d$ over which the averages are performed. Also shown are the elastic domain $\Omega_e$ and the unloading damaged domain $\Omega_{du}$.

We then define the homogenized stresses and strains as the volume averages of the microscopic stresses and strains, respectively, over $\Omega_d$

\[
\langle \sigma \rangle_{\text{dam}} = \frac{1}{|\Omega_d|} \int_{\Omega_d} \sigma_m d\Omega
\]

\[
\langle e \rangle_{\text{dam}} = \frac{1}{|\Omega_d|} \int_{\Omega_d} e_m d\Omega
\]

We refer to this averaging scheme as the failure zone averaging scheme. Since the above domain integrals cannot be converted to surface integrals along $\Gamma_m$, they are computed directly using numerical quadrature. This averaging will filter out the linear contribution which makes the standard stress-strain diagrams sample size dependent.

**Remark 4.2.1.** Somehow similar approaches in the context of micromechanics can be found in the works of [41, 153] in which the stresses and strains are averaged over a three-dimensional homogeneous elastic media containing either randomly oriented or parallel micro cracks.

As an example to test the above averaging scheme, we consider three unit cells of a material with a simple microstructure shown in Figure 4.14. The standard stress-strain curves are given in Figure 4.15a whereas the failure homogenized stress-strain diagrams are shown in Figure 4.15b. Obviously one would conclude that there is no unique size of an RVE while looking at Figure 4.15a. It is, however, clear that an RVE does exist if Figure 4.15b has
4.2 Representative volumes and averaging techniques

Figure 4.14 Unit cells of regular microstructure under uniaxial tension in horizontal direction. Length units are in mm.

been used as the decision criterion. It should be noticed that Equation (4.4) should be used only after development of a failure band i.e., after the peak. That explains the absence of a linear branch in the curves shown in Figure 4.15b.

Figure 4.15 Response of unit cells of regular microstructure: a comparison between the standard averaging and the newly proposed failure zone averaging.

Figure 4.16 plots the evolution of the damaging area $|\Omega_d|$ against the failure averaged normal strain. Note that due to the nonlocal damage model used in this work (see Chapter 2, Section 2.2.1) the localization band becomes wider even at the late stage of failure. That explains the increase of the area of the active damaged domain $|\Omega_d|$ in time as observed in Figure 4.16. Localization zones, however, tend to shrink to a discrete crack i.e., $\Omega_d$ decreases as softening proceeds. This behaviour can be achieved by us-
ing more advanced nonlocal or gradient damage models (see e.g., [52]) for which the proposed failure zone averaging still applies. An attempt was also made in which the domain $\Omega_d$ was on purpose incorrectly defined as $\Omega_m \setminus \Omega_e$ (the symbol $\setminus$ is the difference operator from the set theory) which is, of course, larger than the correct active damaged domain $\Omega_d$ as defined in Equation (4.3) and Figure 4.17 depicts the resulting stress-strain curves which are again sample size dependent, although to a smaller extent than for a standard averaging according to Equation (4.1). Note that we have intentionally included the linear part of the curves to emphasize that the failure zone averaging scheme should be used after localization has occurred.

![Figure 4.16](image) Evolution of the damaging area $|\Omega_d|$ against the failure averaged normal strain.

### 4.2.3 Representative simulations

The application of the newly proposed failure zone averaging scheme to the five samples of heterogeneous material, see Figure 4.2, is given in Figure 4.18 together with the result obtained with the standard averaging method. The curves obviously show that, by filtering out the linear responses in the sample i.e., the stresses and strains in $\Omega_m \setminus \Omega_d$ via the failure zone averaging, the responses are independent of the sample size.

In literature a variety of criteria has been adopted in the statistical analysis of the RVE size namely the slope of the stress-strain curve [58, 60], the dissipated energy [91, 177] and the peak load [177]. In our subsequent statistical analysis we utilize the dissipated energy $G_f$ which is the area under the stress-strain curve
4.2 Representative volumes and averaging techniques

Figure 4.17 Size-dependent response of three samples made of regular microstructure: the failure zone averaging scheme with $\Omega_\text{d}$ incorrectly defined as $\Omega_\text{m} \setminus \Omega_\text{e}$.

\[
G_f = \int_a^b \langle \sigma \rangle_{xx} d \langle \epsilon \rangle_{xx}
\]

(4.5)

where the integration limits $a$ and $b$ for the stress-strain curves obtained with the standard averaging scheme are 0 and $0.2 \times 10^{-3}$, respectively see Figure 4.18a. For those computed using the new failure zone averaging scheme, the integration limits $a$ and $b$ are, respectively, the peak value and $1.5 \times 10^{-3}$, see Figure 4.18b.

The stress-strain diagrams obtained with the proposed failure averaging scheme of four realizations per sample for the five sample sizes (see Figure 4.2) corresponding to $\rho = 45\%$ are given in Figure 4.19. Those obtained with the standard averaging are not reproduced here since they were given in [58, 60]. These curves are the input for the subsequent statistical analysis with the expectation and the standard deviation of a variable $x$ (herein $G_f$) given by

\[
\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i
\]

\[
s = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2
\]

(4.6)

with $n$ being the number of realizations for each sample and $x_i$ is the variable associated with the sample $i$. 

Chapter 4 On the existence of representative volumes for softening materials

The statistical analysis result is given in Figure 4.20 in which the left figure is a reproduction of the result reported in [58, 60] for the sake of comparison. In Figure 4.20a we can see that the deviation converges upon increasing sample size, the expectation however steadily decreases which again demonstrates the RVE size dependence. Figure 4.20b shows, however, that the expectation is stable while the deviation shows a decreasing tendency upon increasing sample size which supports the RVE size independence of the failure zone averaging method. In Figure 4.21, the results for $\rho = 30\%$ and $\rho = 60\%$ are given which shows the same trend.

Figure 4.18 Response of various samples made of random microstructure ($\rho = 45\%$).
4.2 Representative volumes and averaging techniques

Figure 4.19 Failure averaged stress-strain curves of realizations of various samples ($\rho = 45\%$).

4.2.4 A note on periodic boundary conditions

In this section, instead of using the standard BCs given in the left figure of Figure 4.7, periodic BCs (right figure of Figure 4.7) are used. It should be emphasized that the aim is not to perform a comparative analysis on those
Chapter 4 On the existence of representative volumes for softening materials

Figure 4.20  Mean value and standard deviation of the dissipated energy (scaled by $10^5$) for $\rho = 45\%$.

Figure 4.21  Response of various samples made of random microstructure for $\rho = 30\%$ (top) and for $\rho = 60\%$ (bottom).
two BCs. Instead we would like to stress the objectivity of the failure zone averaging technique with respect to the BCs. To this end, only $\rho = 45\%$ is considered and five samples (one realization per sample) are analyzed. The results given in Figure 4.22 indicate that with the failure zone averaging scheme responses which are independent of the micro sample size are obtained also for periodic BCs.

![Response of samples made of random microstructure ($\rho = 45\%$) with periodic boundary conditions.](image)

**Figure 4.22** Response of samples made of random microstructure ($\rho = 45\%$) with periodic boundary conditions.

### 4.2.5 Preliminary result for shear loading

This section discusses the analyses for five samples (one realization per sample) in case of $\rho = 45\%$ subjected to a shear loading as shown in Figure 4.23. The result shown in Figure 4.24 confirms the independence of the homogenized responses obtained with the proposed averaging scheme with respect
to the micro sample size. Although this is a promising result, we believe that a statistical analysis as performed for the uniaxial tension test is needed before a claim on the existence of an RVE for softening materials in shear can be stated.

Figure 4.23 Micro sample subjected to a shear loading.

Figure 4.24 Responses of samples made of random microstructure ($\rho = 45\%$) in shear loading.

(a) standard averaging  (b) failure averaging
4.3 Concluding remarks

In this chapter the issue of existence of the representative volume element for softening quasi-brittle materials with random microstructure has been studied. By performing the averaging over the active damaged domain, rather than over the entire domain, by which the linear contribution has been filtered out, convergence of the stress-strain diagrams for different RVE sizes of softening granular materials has been obtained for tensile loading. The proof of existence of an RVE for softening materials represents a necessary starting point for the hierarchical multiscale scheme for softening materials based on computational homogenization techniques.

As a byproduct of the proposed averaging method, objective homogenized stress-strain relationships which look like traction-separation laws have been obtained. Therefore, the method presented in this chapter could be utilized either in numerical homogenization based multiscale methods or in computational homogenization based methods for macroscale crack modelling. According to the former, a traction-separation law, which is obtained from microscale FE computations via the proposed averaging method in a pre-processing step, is used for describing the behaviour of cracks in a macroscale discrete crack FE model. In the latter, the traction-separation law for a macro crack is determined on the fly, in the spirit of the FE$^2$ method [48], from the responses in a propagating damaged zone at the microscale. This computational homogenization based multiscale crack model is the subject of the next three chapters.
Chapter 5

Multiscale crack modelling: theory *

In Chapter 4, the existence of an RVE for quasi-brittle materials (under tensile loading) with a random complex heterogeneous microstructure exhibiting diffusive damage has been confirmed based upon a new averaging scheme, the failure zone averaging scheme, which filters out the linear contribution of the micro sample.

In this chapter, on the basis of the result presented in Chapter 4, we are going to derive macroscopic cohesive laws, which are objective with respect to micro sample size (assuming the size is sufficiently large), for softening materials with a random heterogeneous microstructure subjected to tensile, shear and mixed-mode loading. It is confirmed that an RVE does exist for softening materials with microstructures undergoing diffusive damage. We also present a computational framework to incorporate those objective cohesive laws in an iterative FE2 setting which is an extension of the approach given in [194] for micro discrete cracking failure to micro diffusive damage fracture. Although similar in some aspects, the major differences between our work and [194] are two-fold. Firstly, the microstructure in this thesis exhibits diffusive damage i.e., we homogenize a macroscopic cohesive law from a microscale localization band. Secondly, the representativeness of the macroscale cohesive law is obtained for materials with a random microstructure and under various loading conditions.

The layout of the chapter is as follows. In Section 5.1, the investigated microstructures and the utilized continuum damage model are given. Section 5.2 presents the standard averaging scheme, the new failure zone averaging technique from Chapter 4 followed by a series of numerical simulations that confirm the existence of an RVE for softening materials. Section 5.3 describes the energetic equivalence theorems to link macroscopic and microscopic models. The multiscale algorithm for adhesive and cohesive cracks is given in Section 5.4 followed by three numerical examples given in Section 5.5.

* Based on reference [135, 137]
5.1 Microstructures and constitutive model

5.1.1 Microstructures

In this chapter, two microstructures are considered. The first one is a simple voided microstructure (radius of the void equals 5 mm) of which three samples with dimensions $20 \times 20$ mm$^2$, $40 \times 20$ mm$^2$ and $40 \times 40$ mm$^2$, as shown in Figure 5.1, will be studied. The second type of microstructure that is analyzed is a random heterogeneous material which is a three-phase material with matrix, aggregates and an interfacial transition zone (ITZ) surrounding each aggregate, see Figure 4.1, Chapter 4. Two samples of dimensions $15 \times 15$ mm$^2$ and $20 \times 20$ mm$^2$, as shown in Figure 5.2, corresponding to 45% aggregate volume fraction are investigated. The size of the aggregates and the thickness of the ITZ are given in Chapter 4. Note that we have not considered bigger samples and different realizations since a statistical analysis of the existence of an RVE for this kind of material has already been given in Chapter 4.

![Figure 5.1](image.png)

Figure 5.1 Three unit cells made of a regular microstructure. All units are in mm.

5.1.2 Constitutive model

Failure of the material is modelled using the gradient enhanced damage model presented in Chapter 2, Section 2.2.1. For the voided microstructure, the material parameters include a Young’s modulus $E$ of 25 000 MPa, Poisson’s ratio $\nu$ of 0.2, damage threshold $\kappa_I$ of $3 \times 10^{-5}$, $\gamma = 0.999$, $\beta = 5000$ and $c = 3.5$ mm$^2$. For the heterogeneous material, the material parameters are given in Table 5.1.
### 5.2 Objective macroscopic cohesive laws

Considering a macro crack with the outward unit normal denoted by \( \mathbf{n} \) and the unit tangent vector represented by \( \mathbf{s} \). A micro sample \( \Omega_m \), which is a rectangle of dimension \( w \times h \), wherein the underlying microstructure is explicitly modelled is associated with every integration point on the macro crack. Let us consider the case in which \( \mathbf{n} \) coincides with \( x_m^i \) see Figure 5.3 for the microscale orthogonal coordinate system. Since the deformation modes of the macro crack include mode I opening and mode II shearing, the boundary conditions (BCs) of the micro model are the ones given in Figure 5.3 for mode I and mode II cases. For mixed-mode problems, BCs are a combination of BCs of mode I and mode II cases. The external boundary of the micro sample is denoted by \( \Gamma_m \) which is composed of \( \Gamma_T, \Gamma_B, \Gamma_L \) and \( \Gamma_R \).

#### Table 5.1 Material parameters of different phases of the random heterogeneous material.

<table>
<thead>
<tr>
<th></th>
<th>Matrix</th>
<th>Aggregate</th>
<th>ITZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E ) [N/mm²]</td>
<td>25 000</td>
<td>30 000</td>
<td>20 000</td>
</tr>
<tr>
<td>( \nu ) [-]</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>( \kappa_I ) [-]</td>
<td>5e-06</td>
<td>0.5</td>
<td>3e-06</td>
</tr>
<tr>
<td>( \gamma ) [-]</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
</tr>
<tr>
<td>( \beta ) [-]</td>
<td>1500</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>( c ) [mm²]</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Figure 5.2 Two micro samples of random heterogeneous material (45% aggregate).
5.2.1 Standard averaging techniques

This section derives the expressions of averaged stresses and strains for a microscopic sample subjected to BCs as shown in Figure 5.3.

The macroscopic homogenized stress $\sigma_M$ is given by (we refer to Chapter 2, Section 2.4)

$$\sigma_M \equiv \frac{1}{wh} \int_{\Omega_m} \sigma_m d\Omega = \frac{1}{wh} \int_{\Gamma_m} t_m \otimes x_m d\Gamma$$

$$= \frac{1}{wh} \int_{\Gamma_R} t_m \otimes (x_R - x_L) d\Gamma + \frac{1}{wh} \int_{\Gamma_T} t_m \otimes (x_T - x_B) d\Gamma$$

(5.1)

where use was made of the anti-periodicity of the tractions. The microscale stress tensor, traction vector and position vector are denoted by $\sigma_m$, $t_m$ and $x_m$, respectively. Quantities associated with the top, bottom, left and right edges of the micro sample are indicated by subscripts T, B, L and R, respectively, see Figure 5.3.

By using the following relations

$$x_R - x_L = wn, \quad x_T - x_B = hs$$

(5.2)

Equation (5.1) becomes

$$\sigma_M = \frac{1}{h} \int_{\Gamma_R} t_m d\Gamma \otimes n + \frac{1}{w} \int_{\Gamma_T} t_m d\Gamma \otimes s$$

(5.3)
5.2 Objective macroscopic cohesive laws

Using the fact that $\mathbf{n}^T = (1, 0)$ and $\mathbf{s}^T = (0, 1)$, the above is simplified to

$$
\sigma_M = \begin{bmatrix}
\frac{f_{R,x}^{\text{int}}}{h} & \frac{f_{T,x}^{\text{int}}}{w} \\
\frac{f_{R,y}^{\text{int}}}{h} & \frac{f_{T,y}^{\text{int}}}{w}
\end{bmatrix}
$$

(5.4)

where $f_{R}^{\text{int}}$ and $f_{T}^{\text{int}}$ are the sum of nodal internal forces along the right and top edges, respectively. Note that the homogenized stress tensor is symmetric due to the rotational equilibrium of the micro sample i.e., $w f_{R,y}^{\text{int}} = h f_{T,x}^{\text{int}}$.

The homogenized strain tensor $\epsilon_M$ is, refer to Section 2.4.2, Chapter 2, given by

$$
\epsilon_M \equiv \frac{1}{w h} \int_{\Omega_m} \epsilon_m d\Omega = \frac{1}{w h} \int_{\Gamma_m} (\mathbf{u}_m \otimes \text{sym} \mathbf{n}) d\Gamma
$$

(5.5)

where the microscale strain tensor and the displacement vector are represented by $\epsilon_m$ and $\mathbf{u}_m$, respectively.

The above can be further elaborated as

$$
\epsilon_M = \frac{1}{w h} \left( \int_{\Gamma_T} [(\mathbf{u}_{m,T}^0 - \mathbf{u}_{m,B}^0) \otimes \text{sym} \mathbf{s}] d\Gamma + \int_{\Gamma_R} [(\mathbf{u}_{m,R}^0 - \mathbf{u}_{m,L}^0) \otimes \text{sym} \mathbf{n}] d\Gamma \right)
$$

$$
= \frac{1}{w} \mathbf{\bar{u}} \otimes \text{sym} \mathbf{n}
$$

(5.6)

where use has been made of the periodicity of the displacement field and the adopted BCs in the last equality. In matrix form, the homogenized strain tensor is given by

$$
\epsilon_M = \begin{bmatrix}
\frac{\bar{u}_x}{w} & \frac{\bar{u}_y}{2w} \\
\text{sym.} & 0
\end{bmatrix}
$$

(5.7)

The macroscopic traction vector $\mathbf{t}_M$ is assumed to be the projection of the macroscopic stress tensor on the crack plane [73, 194]. Using Equation (5.4) this becomes
Chapter 5 Multiscale crack modelling: theory

\[ \mathbf{t}_M \equiv \sigma_M \cdot \mathbf{n} = \frac{\mathbf{f}_R}{h} \] \hfill (5.8)

The homogenized stress-strain (\(\sigma_M^x, e_M^x\)) curves as well as the traction-displacement (\(t_M^x, \bar{u}_x\)) diagrams of the three voided samples (see Figure 5.1) subjected to a tensile loading are given in Figure 5.4. The result on the left shows that for bulk homogenization, the linear elastic response is objective to the micro model size (due to the fact that the elastic slope of the stress-strain curves is the Young’s modulus \(E\) in one dimension). The softening branches are, however, micro model size dependent. For interface homogenization [2, 91] (by interface homogenization, the homogenized quantities are the traction and the displacement of the right edge, see Chapter 2, Section 2.5.1), the linear response is inversely proportional to the width of the sample i.e., being \(E/w\) for one dimensional problems. Obviously, both bulk and interface homogenizations based on standard averaging theorems give results which are not objective to the micro sample size. Figure 5.5 shows the damage distribution in the samples.

\[ \begin{align*}
\text{Figure 5.4} & \quad \text{Three voided samples in tension: bulk vs interface homogenization.} \\
\end{align*} \]

Remark 5.2.1. We have introduced a numerical imperfection to trigger localization at the left voids in samples \(40 \times 20 \text{ mm}^2\) and \(40 \times 40 \text{ mm}^2\), see Figure 5.5. Note that our target material is a brittle random heterogeneous material, Figure 5.2, of which failure is accompanied with the occurrence of one propagating localization band, see Figure 5.14 (no numerical imperfection is needed here). The voided microstructure merely serves as an exemplary material to illustrate our ideas with very low computational cost. The
5.2 Objective macroscopic cohesive laws

Figure 5.5 Damage patterns of three samples under horizontal tensile loading.

The introduction of artificial imperfections for voided samples is just to mimic the behaviour of real random heterogeneous materials. Note that the $40 \times 20 \text{ mm}^2$ and $40 \times 40 \text{ mm}^2$ samples have the same bifurcated solutions, thus the same homogenized response. The $20 \times 20 \text{ mm}^2$ sample captures a different bifurcated path, thus a different homogenized response, Figure 5.4. However, as demonstrated in Chapter 4 (see also Figure 5.6b), the homogenized macroscopic response is size-independent when a proper averaging technique is used even though the samples follow different bifurcation paths. The discussion of bifurcated solutions at the microscale is beyond the scope of this manuscript. Refer to [109] for a related discussion.

5.2.2 Failure zone averaging technique

In Chapter 4 the failure zone averaging technique was presented of which the basic idea is to do the averaging over the active damaged domain $\Omega_d$ rather than over the entire micro domain.

In Figure 5.6 the homogenized stress-strain diagrams of the three voided samples (see Figure 5.1) obtained with the standard averaging scheme (left) and the new failure zone averaging method (right) are given. Figure 5.6a clearly demonstrates that for the softening regime there is no unique size of an RVE– a result reported in [58, 60]. However, Figure 5.6b shows that the stress-strain curves are independent of the micro sample size which in turn means that there exists an RVE for softening materials if the stresses and strains have been defined using the proposed failure zone averaging.
Chapter 5 Multiscale crack modelling: theory

5.2.3 Traction-separation law

In the previous section we have demonstrated that, by performing the averaging over the active damaged domain $\Omega_d$ (refer to Chapter 4, Section 4.2), homogenized stress-strain curves can be obtained which are objective with respect to micro sample size. In what follows, we are going to present a method to extract a macroscopic cohesive law from the microscopic response in the active damaged domain which is independent of the micro sample size.

To this end, let us first define the displacements due to damage $u_{\text{dam}}$ (hereafter referred to as damage displacements) as follows

$$u_{\text{dam}} = \langle e \rangle_{\text{dam}} \cdot (l n)$$

(5.9)

where $l$ is the averaged width of the localization band which is equal to $|\Omega_d| / h$, see Section 5.3 for the definition of $l$ and $\langle e \rangle_{\text{dam}}$ is the failure zone averaged strains defined in Equation (4.4).

Figure 5.7 plots the traction versus the damage displacements $(t^x_M, u^x_{\text{dam}})$ curves for the three voided samples in tension which are obviously independent of the sample sizes. It should be noticed that this conclusion applies only for the portion of the curves after the peak. We therefore define the macro crack opening $[u]_M$ as the damage displacements $u_{\text{dam}}$ shifted to the left by an amount of $\dot{u}_{\text{dam}}$ which is the damage displacements corresponding to the maximum traction

$$[u]_M = u_{\text{dam}} - \dot{u}_{\text{dam}}$$

(5.10)
to obtain initially rigid macroscopic traction-opening relations.

Figure 5.8 reveals the fact that the traction-opening \((t_M^t, 1)\) relation is unique regardless of the sample size which is a result recently reported by [194] for microstructures exhibiting discrete cracking. Note the similarity of Equation (5.10) with Equation (19) in [194] that defines the macro opening displacement as the non-elastic part of the micro displacement. However, the result here holds for a continuum damage model which is relevant for many softening materials.

**Figure 5.7** Three voided samples in tension: traction vs. normal damage displacement \(u_{\text{dam}}^t\).

**Figure 5.8** Traction vs. crack opening displacement diagrams. Left: standard one (computed directly from Equation (5.9)) and right, shifted one obtained with Equation (5.10).

At first glance this result might seem surprising since the traction \(t_M^t\) reflects the tensile stress level over the whole micro sample while the failure displacement \(u_{\text{dam}}\) is only evaluated at the area of damage growth. Nevertheless, it can be explained in a rigorous manner by a proper energetic equivalence theorem which is given in Section 5.3.
5.2.4 Samples under shear and mixed mode loading

The above analysis is repeated now for the same samples but under shear loading, refer to Figure 5.9 for the damage distribution on the deformed configuration.

**Figure 5.9** Damage patterns of three voided samples under shear loading (magnification factor of 50).

**Figure 5.10** Behaviour of three voided samples under shear loading. In the first row, standard homogenization for bulk and crack whereas in the second row, failure zone averaging scheme for bulk and crack.
The results for shear loading are given in Figure 5.10 in which the top figures show results corresponding to the standard averaging scheme whereas the bottom figures show the responses obtained with the failure zone averaging scheme. It is observed once again that using the standard averaging technique, both stress-strain (bulk homogenization) and traction-separation (interface homogenization) diagrams are sample size dependent. However, when the failure zone averaging scheme is used, both the stress-strain and traction-separation curves are independent of the sample size or equivalently an RVE does exist for softening materials under shear loading.

Next, mixed mode loading (a displacement $(\bar{u}_x, \bar{u}_y)$ with 1:1 proportion was imposed on the right edge of the micro sample) has also been performed for these three samples of which the results are given in Figure 5.11. The first row shows the result of mode I whereas the second row gives the behavior of mode II. It is observed once again that the traction-separation curves are independent of the sample size.

![Figure 5.11](image)

**Figure 5.11** Three voided samples under mixed mode loading: standard averaging (left) versus failure zone averaging (right), for the $x$-component (top) and for the $y$-component (bottom).
5.2.5 Existence of an RVE for materials with random microstructure

The analysis is finally applied to the two samples with random complex microstructure, see Figure 5.2, for both tensile and shear loading conditions. The results given in Figure 5.12 and Figure 5.13 confirm the independence of the homogenized response with respect to the sample size (when this size is sufficiently large in order for the micro sample to contain enough microstructural constituents) if the failure zone averaging was used to extract only the inelastic responses occurring in the samples. For shear loading further studies for more samples in combination with a statistical analysis would be necessary to prove the applicability of the proposed averaging technique. In Figure 5.14 typical damage patterns in the samples are given.

![Figure 5.12](image)

(a) stress-strain

(b) traction-opening

**Figure 5.12** Bulk (a) versus crack homogenization (b) for random microstructure under tensile loading.

5.3 Energetically equivalent macro/micro coupling

Fracture can occur inside the bulk of the material or along the interface between two different materials. For the former, the fracture surface is termed a cohesive crack whereas for the latter, the term adhesive (or interfacial) crack is used. For the case of cohesive cracks, homogenization is applied to a finite element model representing the bulk material around the crack. In the case of adhesive cracks, the adopted micro model represents the material in the adhesive layer. This section develops the link between macro and micro models for both cohesive and adhesive cracks.
5.3 Energetically equivalent macro/micro coupling

Figure 5.13 Bulk (a) versus crack homogenization (b) for random microstructure under shear loading.

Figure 5.14 Damage patterns in random heterogeneous samples under tension. Note that the failure bands are periodic.

5.3.1 Cohesive cracks

In Section 5.2.2 the objectivity of the \( (\langle \sigma \rangle_{\text{dam}}, \langle \varepsilon \rangle_{\text{dam}}) \) curves has been demonstrated via numerical examples. We have shown that the \( (t_M, u_{\text{dam}}) \) diagrams are independent of the micro sample size as well. In what follows, we are going to prove mathematically the representativeness of \( (t_M, u_{\text{dam}}) \) diagrams providing the objectivity of \( (\langle \sigma \rangle_{\text{dam}}, \langle \varepsilon \rangle_{\text{dam}}) \) curves (which have been demonstrated extensively in Chapter 4, see also Figure 5.6). To this end, we need to prove the following equation

\[
lh(\langle \sigma \rangle_{\text{dam}} : \langle \varepsilon \rangle_{\text{dam}}) = h(t_M \cdot u_{\text{dam}}) \quad (5.11)
\]
where the left hand side is the energy dissipated in the active damaged zone $\Omega_d$ and the right hand side is the dissipated energy of the equivalent macro crack. Note that $l$ is the width of the equivalent failure band which is equal to $|\Omega_d|/h$, see Figure 5.15. Note that this expression was obtained for the case in which the localization band cuts the micro sample at two points, one on the lower edge and the other on the upper edge. This is a valid assumption considering mode I failure studied in this work.

![Figure 5.15](image)

**Figure 5.15** From a microscale localization band to a macroscale equivalent crack via an energetic equivalence consideration.

The proof of the above is as follows. The right hand side of Equation (5.11) can be elaborated as

$$h(t_M \cdot u_{\text{dam}}) = \langle \sigma'_{\text{dam}} \cdot n \rangle \cdot \langle \epsilon'_{\text{dam}} \cdot n \rangle |lh$$

$$= \sigma'_{\text{dam}} \epsilon'_{\text{dam}} \eta_j n_k |lh$$

$$= \sigma'_{\text{dam}} \epsilon'_{\text{dam}} \delta_{jk} |lh = \sigma'_{\text{dam}} \epsilon'_{\text{dam}} |lh$$

(5.12)
where use was made of Equation (5.9) and the fact that $t_M$ equals $\langle \sigma \rangle_{\text{dam}} \cdot n$ due to equilibrium, see Figure 5.16. In the above, $\delta_{jk}$ is the Kronecker delta tensor$^*$. Comparing the above with the left hand side of Equation (5.11) concludes the proof. According to Figure 5.15, this proof corresponds to the transition from the equivalent failure band to the crack.

Applying the Hill-Mandel theorem [71] to the active damaged domain $\Omega_d$ yields

$$
\frac{1}{|\Omega_d|} \int_{\Omega_d} \sigma_m : \delta \varepsilon_m d\Omega = \langle \sigma \rangle_{\text{dam}} : \delta \varepsilon_{\text{dam}}
$$

Note that the above equation was obtained by considering $\Omega_d$ as an independent domain. Since a mathematical proof of the above equation is missing, we present numerical evidence of the validity of Equation (5.13) in Section 5.3.3. Using Equation (5.11), Equation (5.13) becomes

$$
\frac{1}{wh} \int_{\Omega_d} \sigma_m : \delta \varepsilon_m d\Omega = \frac{1}{w} t_M \cdot \delta \varepsilon_{\text{dam}}
$$

The LHS of the above can be written as the difference between the virtual work of the whole micro sample and the linear virtual work. Therefore, we can write

$$
\frac{1}{wh} \int_{\Omega_m} \sigma_m : \delta \varepsilon_m d\Omega - \frac{1}{wh} \int_{\Omega_l} \sigma_m : \delta \varepsilon_m d\Omega = \frac{1}{w} t_M \cdot \delta \varepsilon_{\text{dam}}
$$

where $\Omega_l$ is the linear domain i.e., $\Omega_l = \Omega_m \setminus \Omega_d$.

Using the virtual work equation for the first term of the above equation and the Hill-Mandel condition for the second term, Equation (5.15) can be rewritten as

$$
\frac{1}{wh} \int_{\Gamma_m} t_m \cdot \delta \varepsilon_m d\Gamma - \frac{w - l}{w} \langle \sigma \rangle_{\text{lin}} : \delta \varepsilon_{\text{lin}} = \frac{1}{w} t_M \cdot \delta \varepsilon_{\text{dam}}
$$

where the homogenized linear stresses and strains $\langle \sigma \rangle_{\text{lin}}$ and $\delta \varepsilon_{\text{lin}}$ are given by

$^*$We have switched the position of the subscript $\text{dam}$ to superscript when indicial notation was used for convenience of reading.
Chapter 5 Multiscale crack modelling: theory

\[
\langle \sigma \rangle_{\text{lin}} = \frac{1}{(w-l)h} \int_{\Omega} \sigma_m \text{d}\Omega \\
\delta(e)_{\text{lin}} = \frac{1}{(w-l)h} \int_{\Omega} \delta e_m \text{d}\Omega
\]  

(5.17)

In order to compute the term \( \langle \sigma \rangle_{\text{lin}} : \delta(e)_{\text{lin}} \), a rectangular homogeneous sample subjected to a traction \( t_M \) on the right edge is considered. The stresses in that sample are given by

\[
\langle \sigma \rangle_{\text{lin}}^{xx} = t_x^M \quad \langle \sigma \rangle_{\text{lin}}^{yy} = 0 \quad \langle \sigma \rangle_{\text{lin}}^{xy} = t_y^M
\]  

(5.18)

The above equation expressed in matrix-vector notation by using Voigt notation becomes

\[
\begin{bmatrix}
\langle \sigma \rangle_{\text{lin}}^{xx} \\
\langle \sigma \rangle_{\text{lin}}^{yy} \\
\langle \sigma \rangle_{\text{lin}}^{xy}
\end{bmatrix} =
\begin{bmatrix}
1 & 0 & t_x^M \\
0 & 0 & t_y^M \\
0 & 1 & t_y^M
\end{bmatrix} \equiv \Delta t_M
\]  

(5.19)

or in tensor notation as

\[
\langle \sigma \rangle_{\text{lin}} = \Delta \cdot t_M
\]  

(5.20)

with the third-order tensor \( \Delta = n \otimes n \otimes n + (n \otimes s + s \otimes n) \otimes s \), which was firstly given in [194].

Now, \( \langle \sigma \rangle_{\text{lin}} : \delta(e)_{\text{lin}} \) can be written as

\[
\langle \sigma \rangle_{\text{lin}} : \delta(e)_{\text{lin}} = \langle \sigma \rangle_{\text{lin}} : D_{\text{lin}}^{-1} : \delta(e)_{\text{lin}} \\
= (\Delta \cdot t_M) : [D_{\text{lin}}^{-1} : (\Delta \cdot \delta t_M)] \\
= \iota_p^M \left[ \Delta_{ijkl} (D_{\text{lin}}^{-1})_{ijkl} \Delta_{klm} \right] \delta t_m^M \\
= \iota_p^M \Delta_{ijkl} (D_{\text{lin}}^{-1})_{ijkl} \delta t_m^M = t_M \cdot C_{\text{lin}} : \delta t_M
\]  

(5.21)
Note that the second-order tensor $\mathbf{C}_{\text{lin}}$ is the projection on the crack plane of the fourth-order compliance tensor $\mathbf{D}_{\text{lin}}^{-1}$ [194]. In the above derivation, the minor symmetry of $\mathbf{D}_{\text{lin}}^{-1}$ was used.

Substituting Equation (5.21) into Equation (5.16) yields

$$
\frac{1}{wh} \int_{t_m} \mathbf{t}_m \cdot \delta \mathbf{u}_m d\Gamma = \frac{w - l}{w} \mathbf{t}_M \cdot \mathbf{C}_{\text{lin}} \cdot \delta \mathbf{t}_M + \frac{1}{w} \mathbf{t}_M \cdot \delta \mathbf{u}_{\text{dam}} \tag{5.22}
$$

or

$$
\frac{1}{w} \mathbf{t}_M \cdot \delta \mathbf{u}_R = \frac{w - l}{w} \mathbf{t}_M \cdot \mathbf{C}_{\text{lin}} \cdot \delta \mathbf{t}_M + \frac{1}{w} \mathbf{t}_M \cdot \delta \mathbf{u}_{\text{dam}} \tag{5.23}
$$

where the boundary conditions shown in Figure 5.3 were adopted to compute the LHS of Equation (5.22). In the above, $\mathbf{u}_R$ is the displacement vector of the right edge of the micro sample. The fact that the above holds true for any $\mathbf{t}_M$ yields

$$
\delta \mathbf{u}_R = (w - l) \mathbf{C}_{\text{lin}} \cdot \delta \mathbf{t}_M + \delta \mathbf{u}_{\text{dam}} \tag{5.24}
$$

which can be rewritten as

$$
\delta \mathbf{u}_R = (w - l) \mathbf{C}_0 \cdot \delta \mathbf{t}_M + \delta \mathbf{u}_{\text{dam}} + \delta \mathbf{u}_M \tag{5.25}
$$

with $\mathbf{C}_0$ being the second-order compliance tensor $\mathbf{C}$ but now evaluated in the undeformed microscale configuration and $\delta \mathbf{u}_M$ given by

$$
\delta \mathbf{u}_M = (w - l) [\mathbf{C}_{\text{lin}} - \mathbf{C}_0] \cdot \delta \mathbf{t}_M \tag{5.26}
$$

After a localization band has been formed, the nonlinear part of the total microscale displacement $\mathbf{u}_R$ is assumed to be completely governed by the damage displacements $\mathbf{u}_{\text{dam}}$. In other words, $\delta \mathbf{u}_M = 0$, hence Equation (5.25) becomes

$$
\delta \mathbf{u}_R = (w - l) \mathbf{C}_0 \cdot \delta \mathbf{t}_M + \delta \mathbf{u}_{\text{dam}} \tag{5.27}
$$

Using Equation (5.10), the equation can be rewritten as follows
\[ \mathbf{u}_R = (w - l) \mathbf{C}_0 \cdot \mathbf{t}_M + [\mathbf{u}]_M + \dot{\mathbf{u}}_{\text{dam}} \] (5.28)

The above equation provides the scale transition relation from microscale responses to the macroscale cohesive law (traction \( \mathbf{t}_M \) and separation \([\mathbf{u}]_M\)). Note that for the case in which the micro sample undergoes discrete cracking \((l = 0)\), Equation (5.28) reduces to Equation (17) given in [194].

5.3.2 Adhesive cracks

There are two ways in which homogenization schemes for an adhesive crack can be developed, see Figure 5.17. They are referred to as case I and case II.

**Figure 5.17** Schematic representation of the homogenization schemes for adhesive cracks with thickness \( t_{\text{adh}} \). Case I refers to micro samples having \( w = t_{\text{adh}} \) whereas Case II corresponds to micro samples having \( w < t_{\text{adh}} \). Periodic BCs are denoted by dashed lines.

**Case I** In this case, the micro model covers the complete thickness of the adhesive crack and thus the displacement of the micro model \( \mathbf{u}_R \) can be directly related to the macro jump via

\[ \mathbf{u}_R = [\mathbf{u}]_M \] (5.29)

The above is used as BCs for the micro model. After solving the micro model, the macro traction \( \mathbf{t}_M \) is given by Equation (5.8), see [2, 194].

**Case II** In case the adhesive crack \( t_{\text{adh}} \) is considerably larger than its microstructural constituents and additionally the geometry in the thickness
direction is periodic, the homogenization can be applied to a micro model having a width smaller than $t_{adh}$. The homogenization relation for a cohesive crack, Equation (5.28) can be modified for the case of an adhesive crack with thickness $t_{adh}$ as follows. When $w = t_{adh}$, we have $u_R = \langle u \rangle_M$, hence Equation (5.28) becomes

$$\langle u \rangle_M = (t_{adh} - l)C_0 \cdot t_M + \langle u \rangle_M + \dot{u}_{dam}$$  \hspace{1cm} (5.30)

solving for $\dot{u}_{dam}$ and substituting it into Equation (5.28) yields

$$u_R = (w - t_{adh})C_0 \cdot t_M + \langle u \rangle_M$$  \hspace{1cm} (5.31)

which provides the homogenization relation between microscale information and the macroscale cohesive law ($t_M$, $\langle u \rangle_M$). Note that this equation resembles Equation (35) in [194].

**Remark 5.3.1.** The result obtained with the case I scheme is referred to as the reference solution. Case II is a homogenization scheme that adjusts the solution of a smaller micro model to match the reference solution. Apparently those homogenization schemes do not use the failure zone averaging technique since the entire response of the micro model is mapped to the macro adhesive crack.

**Remark 5.3.2.** Since both homogenization schemes, presented as case I and case II, should yield the same result, one might argue that case I is sufficient. The use of case II, however, offers the following benefits

- a smaller micro sample results in less computational efforts;
- a smaller micro sample could minimize the possibility of microstructural snapback appearances, thus increases the robustness of the method.

### 5.3.3 Numerical verification of Equation (5.13)

Equation (5.13) can be rewritten as $\langle \sigma_m : \delta \epsilon_m \rangle_{dam} = \langle \sigma \rangle_{dam} : \delta \langle \epsilon \rangle_{dam}$ which states that the volume average (over $\Omega_d$) of the microscopic work equals the work done by the averaged (over $\Omega_d$) stresses and strains. Although this equation bears similarity with the Hill-Mandel theorem which is used
in standard homogenization schemes, we are currently unable to provide a rigorous proof for it. Instead, we present numerical evidences of the satisfaction of Equation (5.13) as shown in Figure 5.18. Two samples, of which one has a periodic microstructure and the other has a random microstructure, are analyzed in a uniaxial tension test. The considered material is the three-phase material described in Section 5.1.1. It is seen that Equation (5.13) is practically verified.

![Figure 5.18 Numerical evidences of Equation (5.13).](image)

### 5.4 Computational multiscale crack modelling

In the previous sections it has been shown that traction-separation laws which are objective to the micro model size (when this size is, for ran-
5.4 Computational multiscale crack modelling

domains materials, larger than a minimum value) are obtained for materials with simple underlying microstructure and complex random microstructure under various loading conditions including tensile, shear and mixed-mode loading. These cohesive laws can be utilized in two ways, either in numerical homogenization schemes or in computational homogenization methods e.g., in a FE setting. According to the former, a micro model with properly chosen dimension which is determined, for example, by the RVE’s size quantification procedure given in [60, 151, 177], is numerically loaded at different loading conditions, the resulting cohesive laws are stored and later on used in a macroscopic FE computations as standard phenomenological constitutive laws. They are known as *micro-mechanically derived cohesive laws*. In the spirit of the latter, there is a direct coupling between macro model and micro models. This section presents computational homogenization schemes for both cohesive and adhesive cracks using the homogenization relations developed in Section 5.3.

**Remark 5.4.1.** The reasons of choosing a computational homogenization approach rather than a numerical homogenization method are as follows. Firstly, the CH approach provides fine scale solutions that enables the quantification of the local stresses and strains in the microstructures. Secondly, the numerical homogenization approach might lose certain details of the fine scale solutions due to, for example, history dependence [92]. This is the case for nonlinear materials especially rate dependent materials.

5.4.1 Adhesive crack homogenization-case I

Homogenization for material layers with $w = t_{adh}$ has firstly been discussed in [110] for small strain problems and later in [73] for the case of finite deformations. In this section, an algorithm for small deformation is given in which a detailed derivation of the tangent matrix is presented. We provide the tangent in a form which is readily incorporated in computer codes (not the case in [73]).

The $2 \times 2$ cohesive tangent matrix $T_M$—the tangent in rate format of the macro cohesive law $\delta t_M = T_M \delta [u]_M$, is determined as follows. For illustration assuming that there are only two nodes on the right edge, the traction rate defined in Equation (5.8) then becomes
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\[
\begin{bmatrix}
\delta f_{x_M} \\
\delta f_{y_M}
\end{bmatrix}
= \frac{1}{h}
\begin{bmatrix}
\delta f_{x_1} + \delta f_{x_2} \\
\delta f_{y_1} + \delta f_{y_2}
\end{bmatrix}
= \frac{1}{h}
\begin{bmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
\delta f_{x_1} \\
\delta f_{y_1} \\
\delta f_{x_2} \\
\delta f_{y_2}
\end{bmatrix}
\tag{5.32}
\]

From the converged linear system of the micro model \( K\delta u = \delta f \), the force along the right edge can be written as \( K^*\delta u_R = \delta f_R \), so the above becomes

\[
\begin{bmatrix}
\delta f_{x_M} \\
\delta f_{y_M}
\end{bmatrix}
= \frac{1}{h}
\begin{bmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
K_{11} & K_{12} & K_{13} & K_{14} \\
K_{21} & K_{22} & K_{23} & K_{24} \\
K_{31} & K_{32} & K_{33} & K_{34} \\
K_{41} & K_{42} & K_{43} & K_{44}
\end{bmatrix}
\begin{bmatrix}
\delta u_{x_1} \\
\delta u_{y_1} \\
\delta u_{x_2} \\
\delta u_{y_2}
\end{bmatrix}
\tag{5.33}
\]

where \( K^* \) is the condensed stiffness matrix according to the degrees of freedom of the nodes along the right edge, see [86] for a discussion on this static condensation procedure. Writing the displacements of the right edge in terms of the macro opening displacement, we can rewrite Equation (5.33) as

\[
\begin{bmatrix}
\delta f_{x_M} \\
\delta f_{y_M}
\end{bmatrix}
= \frac{1}{h}
\begin{bmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
K_{11} & K_{12} & K_{13} & K_{14} \\
K_{21} & K_{22} & K_{23} & K_{24} \\
K_{31} & K_{32} & K_{33} & K_{34} \\
K_{41} & K_{42} & K_{43} & K_{44}
\end{bmatrix}
\begin{bmatrix}
\delta u_{x_R} \\
\delta u_{y_R} \\
\delta u_{x_1} \\
\delta u_{y_1}
\end{bmatrix}
\tag{5.34}
\]

which obviously shows that the macro cohesive tangent matrix is given by

\[
T_M = \frac{1}{h} M^T K^* M
\tag{5.35}
\]

Upon convergence of the micro FE model, the micro stiffness matrix \( K \) is statically condensed out to obtain the right edge micro stiffness matrix \( K^* \) and finally the above equation gives the macro cohesive tangent matrix.
For an iteration of a macroscopic load step, the procedure to compute the macro traction and macro cohesive tangent providing a macro opening displacements $[u]_M$ is given in Box 3.

**Box 3 Adhesive crack homogenization-case I.**

1. Given $[u]_M$
2. Compute $u = [u]_M$
3. Apply that displacement $u$ on the RVE’s right edge
4. Solve the RVE problem *
5. Compute the macro traction using Equation (5.8)
6. Compute the macro tangent using Equation (5.35)
7. Go back to macro model and proceed as in standard FE
8. Upon macro model convergence, commit the state of all micro models

* With its state (displacement and internal variables) being reset to its previous converged values.

### 5.4.2 Adhesive crack homogenization-case II

Given the macro opening displacements $[u]_M$, the dimension $(w, h)$ of the micro model and the adhesive thickness $t_{adh}$, the system of equations that we want to solve for $u_m$ and $t_M$ is the following

\[
\begin{align*}
    f_{\text{int}}(u_m) &= f_{\text{ext}}(t_M) \\
    u_R(u_m) &= [w - t_{adh}]C_0t_M + [u]_M
\end{align*}
\]

(5.36a) (5.36b)

In words, solving the micro equilibrium Equation (5.36a) while satisfying the homogenization relation Equation (5.31). In the above, $f_{\text{int}}$ and $f_{\text{ext}}$ are the micro internal and external force vectors, respectively.

In [194] the above system was solved simultaneously for $u_m$ and $t_M$. This means that the sought-for macro traction $t_M$ is the external force applied
on the right edge of the micro sample and Equation (5.36b) is similar to the constraint equation in arc-length control methods. The method can therefore be considered as a direct force-control computational homogenization method for crack modelling. In the current implementation, we follow a displacement-control procedure, as presented in the sequel.

We model the elastic behavior of the crack as follows. Denoting the thickness of the macro crack \( t_{adh} \), then the displacement imposed on the micro model reads \( u_R = \left( \frac{w}{t_{adh}} \right) \mathbb{u}_M \). Note that the tangent given in Equation (6.12b) in this case is scaled by a factor of \( w/t_{adh} \). In this way, the macro linear response will be objective to the micro sample size. The proof of the relation \( u_R = \left( \frac{w}{t_{adh}} \right) \mathbb{u}_M \) in the linear regime is as follows. In terms of displacements, Equation (5.36b) is rewritten as

\[
\mathbf{u}_R = \frac{w - t_{adh}}{w} \mathbf{u}_{lin} + \mathbb{u}_M = \frac{w - t_{adh}}{w} \mathbf{u}_R + \mathbb{u}_M \tag{5.37}
\]

where the fact that \( \mathbf{u}_{lin} = \mathbf{u}_R \) has been used. Solving the above equation for \( \mathbf{u}_R \) yields

\[
\mathbf{u}_R = \frac{w}{t_{adh}} \mathbb{u}_M \tag{5.38}
\]

which concludes the proof.

Whenever the peak at the micro model is observed, say by an appearance of one negative eigenvalue of the macro tangent \( \mathbf{T}_M \) as proposed in [108], we switch to the use of the algorithm given in Box 4 as a kind of multiscale constitutive box for the softening branch. As can be seen, this scheme is an iterative displacement-control computational homogenization scheme for modelling cracks. It should be emphasized that the iterative procedure converged in the numerical simulations presented here. The appealing point of the iterative scheme compared to the force-control scheme given in [194] is that at micro level, a standard FE procedure is readily reused which facilitates the incorporation of the method in existing FE codes.

In Box 4, \( \varepsilon \) is the convergence tolerance and \( \mathbf{D}_0 \) is the homogenized elasticity matrix which is computed, in a pre-processing step i.e., before the multiscale problem starts, using the standard bulk homogenization method (see Section 2.4).
5.4 Computational multiscale crack modelling

Box 4 Iterative scheme for adhesive crack-case II homogenization.

1. Given $[[u]]_M$ and $u_{lin}^0$

2. Compute $\bar{u}_R = [[u]]_M + \left( \frac{w - t_{adh}}{w} \right) u_{lin}^0$

3. Apply that displacement $\bar{u}_R$ on the RVE’s right edge

4. Solve the RVE problem

5. Compute the macro traction $t_M$ using Equation (5.8)

6. Compute $u_{lin} = wC_0t_M$, with $C_0 = \Delta^T D_0^{-1} \Delta$

7. Check convergence
   a) compute $u_R = \frac{w - t_{adh}}{w} u_{lin} + [[u]]_M$
   b) check $||u_R - \bar{u}_R|| < \varepsilon ||u_R||$. If no, go back to step 2 with $u_{lin}^0 = u_{lin}$. Else, proceed to step 8

8. Compute the macro material tangent using Equation (5.35)

9. Upon macro model convergence, commit the state of all micro models

* Superscript 0 denotes quantities of the previous converged macroscopic load step.

5.4.3 Cohesive crack homogenization

The system of equations that needs to be solved for $u_m$ and $t_M$, given the macro jump $[[u]]_M$ and the compatibility displacement $\bar{u}_{dam}$, is

\[ f_{int}(u_m) = f_{ext}(t_M) \]
\[ u_R(u_m) = [w - l(u_m)]C_0t_M + [[u]]_M + \bar{u}_{dam} \]

which consists of the micro equilibrium equation and the homogenization relation Equation (5.28).

Similar to the case of adhesive cracks (case II scheme) presented in the previous section, the above system is solved by an iterative displacement-control procedure as given in Box 5. This is not only because both adhe-
sive and cohesive cracks can be handled in a common displacement-control framework but also due to the dependency of the localization band width \( l \) on the micro displacements \( \mathbf{u}_m \). Since the macroscopic bulk is not coupled to an RVE here (in Chapter 7 the multiscale scheme is also used for coupling the bulk material to a microstructure), the initiation/propagation of macro-cracks must be based on a macroscopic failure criterion. The maximum principal stress criterion (e.g., [198]) has been used for the crack initiation/propagation. The crack direction is determined based on the macroscopic stresses as normally done in standard cohesive crack modelling. The iterative displacement-control procedure for cohesive cracks is summarized in Box 5.

In Box 5, the macroscopic maximum principal stress is denoted by \( \sigma_1 \) and \( \sigma_{\text{ult}} \) is the ultimate strength of the material which is, in a multiscale framework, the ultimate load of the microscale model. This quantity is currently determined by loading first the micro sample in a pre-processing step (see Chapter 6, Section 6.2.1 for details). The crack initiation equation \( \sigma_1 \geq \alpha \sigma_{\text{ult}} \), \( \alpha \approx 1.0 \), as proposed by [194], ensures that step 3b in Box 5 succeeds i.e., no divergence occurs. The proposed algorithm can be incorporated in any numerical code with the capacity to model cohesive cracks e.g., PUM-based enrichment finite elements [124, 198].

The macroscopic bulk behaves elastically with effective properties computed based on numerical homogenization applied to the micro samples. Given the strain vector, the macroscopic stress vector is thus simply given by

\[
\sigma_M = \mathbf{D}_0 \mathbf{e}_M
\]  

without resorting to a microscale computation. This dramatically reduces the computational cost of the multiscale scheme.

### 5.4.4 Some algorithmic aspects

For a robust and efficient implementation of the proposed multiscale framework, some algorithmic aspects have to be considered. Since in [194] related details have already been given, in this section we only discuss some techniques that ensure a robust multiscale scheme. It is likely that in a FE\(^2\) simulation divergence of one (or more) micro problem(s) will occur. Straightforward remedies of this problem could be either (i) resolving the macro
Box 5 Iterative displacement-controlled homogenization for cohesive cracks.

1. Initialization: compute $D_0, C_0 = \Delta^T D_0^{-1} \Delta, \sigma_{ult}$

2. Run macro model until $\sigma_I \geq \alpha \sigma_{ult}, \alpha \approx 1.0$

3. Insert a crack segment with a proper direction
   a) Initialize 2 micro models associated with 2 GPs on crack segment
   b) Loading those 2 micro models up to $\sigma_I$ via load control *
   c) Computing the initial damage displacements $\hat{u}_{dam}$

4. Given $\|u\|_M, u_0^{lin}$ and $l^0$
   a) Compute $\bar{u}_R = [u]_M + \hat{u}_{dam} + \left(\frac{w - l^0}{w}\right) u_0^{lin}$
   b) Apply that displacement $\bar{u}_R$ on the RVE’s right edge
   c) Solve the RVE problem
   d) Compute the macro traction $t_M$ using Equation (5.8)
   e) Compute $u_{lin} = w C_0 t_M$
   f) Compute the new localization band width $l = |\Omega_d| / h$
   g) Check convergence
      i. compute $u_R = [u]_M + \hat{u}_{dam} + \frac{w - l}{w} u_{lin}$
      ii. check $||u_R - \bar{u}_R|| < \epsilon ||u_R||$. If no, go back to step 3b with $\hat{u}_R = u_R$. Else, proceed to step 4

5. Compute the macro material tangent using Equation (5.35).

6. Upon macro model convergence, commit the state of all micro models

* This is achieved by subdividing $\sigma_I$ into a number of small load steps.
considered. Needless to say, a comparison study, say by means of numerical experiments, of those techniques would be necessary to choose the most efficient one and this is a topic of further study. It is emphasized that the proposed scheme cannot deal with the snapback behavior occurring at the micro models\(^\dagger\). Macroscopic snapback can however be handled by, for instance, the energy-based arc-length control given in \([67, 193]\). This issue will be presented in Section 6.3.5, Chapter 6.

Details on the computer implementation of the presented multiscale crack models in the Jem/Jive C++ library have been reported in \([132]\).

### 5.5 Benchmark problems

In this section, three numerical examples are given. The first two examples aim to verify the objectivity of the macroscopic response with respect to the micro sample size. In the last example, a verification of the proposed multiscale models against a direct numerical simulation is provided. Note that this section only presents simple proof-of-concept examples. More complex examples will be given in the next chapter.

#### 5.5.1 Adhesive crack

Figure 5.19 gives a benchmark problem for verifying the proposed multiscale scheme. The aim is to check whether the macroscopic response is objective to the micro sample size. The material parameters of the micro model are given in Section 5.1.2. The macro bulk material is an elastic material with Young’s modulus of 25,000 N/mm\(^2\) and Poisson’s ratio of zero. Note that in contrary to the cohesive crack, for an adhesive crack, the macroscopic bulk is not related to the microstructure of the adhesive crack. A plane stress condition is assumed for the macro model and the micro models as well. The thickness of the interface \(t_{\text{adh}}\) is assumed to be 40 mm.

Using the case I adhesive crack homogenization scheme given in Box 3, the macroscopic load-displacement diagrams corresponding to the 40×20 and 40×40 samples (note that the sample 20×20 cannot be used in this case since its width is smaller than \(t_{\text{adh}}\)) are given in Figure 5.20-left. The responses are obviously independent of the micro sample size. Figure 5.20-right presents the macroscopic responses for all three samples using the new

\(^\dagger\)It is, however, noticed that snapback is not likely to occur in the micro samples.
5.5 Benchmark problems

Figure 5.19 Crack modelling by interface elements. Cohesive law extracted from micro FE computations whereas bulk material obeys a phenomenological linear elastic constitutive law.

Figure 5.20 Adhesive crack benchmark problem: macroscopic load displacement ($\bar{u}$) curves obtained with the standard scheme (left) and the iterative displacement-control homogenization scheme (right). Top figures correspond to ductile fracture ($\beta = 3000$) and the bottom ones for brittle fracture ($\beta = 5000$).
iterative homogenization scheme given in Box 4. The results practically coincide. It has been observed that for one macroscale Newton-Raphson iteration, the iterative scheme (Box 4) converges in two to four iterations with a tolerance of $c = 10^{-4}$. Far from the peak, when the contribution of elastic processes becomes negligible, the number of required iterations usually is only one or two. We refer to the next chapter for a numerical study of the convergence characteristic of the iteration scheme given in Box 4.

### 5.5.2 Cohesive crack

Figure 5.21 depicts a simple crack growth simulation problem, a bar in uniaxial tension which is discretized by 3 four-noded quadrilateral elements. Refer to Section 5.1.2 for the material parameters of the micro models (except $\beta = 1000$). When the maximum principal stress in the bar exceeds 0.4475 MPa (i.e., 95% of the micro model ultimate load $\sigma_{\text{ult}}$), a vertical crack is, due to symmetry, inserted in the middle element. The behavior of that crack is governed by one of the three microstructures as shown in Figure 5.21. A plane stress condition is assumed for the micro models. The aim of the example is to verify the objectivity of the macroscopic responses with respect to the utilized microstructures.

![Figure 5.21](image.png)

**Figure 5.21** Cohesive crack modelling by PUM with cohesive law coming from microscopic FE computations. Due to symmetry, a vertical crack (dashed line) is inserted in the middle element upon violation of the fracture criterion. All units are in mm.

Figure 5.22 presents the macroscopic load-displacement ($\bar{u}$) curves which are clearly independent of the microstructures used to obtain the homogenized macroscopic cohesive laws shown in the right figure. Note that since
5.5 Benchmark problems

Figure 5.22 Cohesive crack problem: objective macroscopic load-displacement diagrams obtained with various microstructures (left) and homogenized traction-opening laws (right).

Figure 5.23 Cohesive crack problem: consequences of the crack initiation moment on the overall macroscopic response (left) and close-up view (right).

The macro crack was inserted slightly before the ultimate load of the micro models, the homogenized cohesive laws are not initially rigid as conventional cohesive models. We have also analyzed the effect of the $\alpha$ parameter used in the crack initiation/propagation criterion $\sigma_I \geq \alpha \sigma_{ult}$ on the overall macroscopic response. The result, reported in Figure 5.23 for the $20 \times 20$ sample, shows that there is hardly any considerable effect of this parameter on the overall behavior of the macroscopic sample.
5.5.3 Verification of the method against DNS

To verify the proposed multiscale method, let us consider the example shown in Figure 5.24 of which the solution obtained with the multiscale model is going to be compared with the one obtained with the DNS (Direct Numerical Simulation). The shaded region of width 20 mm is modelled as a damageable material (material parameters can be found in Section 5.1.2 except $\beta = 3000$) whereas the rest behaves elastically. The finite element mesh of the DNS model is given in Figure 5.25.

In case that the shaded region represents the microstructure of a material layer of thickness $t_{adh} = 20$ mm, the finite element mesh for the multiscale model (adhesive crack-case I) is given in Figure 5.26. The adequacy of the multiscale solution can be judged from Figure 5.27 which presents the comparison of load-displacement curves between the multiscale (denoted as FE2) simulation and the DNS. The multiscale solution captures the peak load and later stages well with a much lower computational time (in this particular example the DNS simulation time is approximately 10 times the one of the multiscale method).

For the multiscale cohesive crack homogenization scheme, the finite element discretizations for the macro and micro models are presented in Figure 5.28. The adequacy of the multiscale solution can be judged from Figure 5.29 which compares the load-displacement curve of the multiscale model to that of the DNS model. The multiscale solution captures the peak load and later
stages well. For this particular case, the DNS simulation required approximately 6 times the computation time of the multiscale model. However it should be stressed that for problems in which the crack path is not known a priori, the use of DNS seems to be impractical since the microstructure has to be resolved everywhere leading to a mesh with extremely high number of elements.
5.6 Concluding remarks

In this chapter macroscopic cohesive laws (both mode I and mode II), which are independent of the micro sample size, were obtained for quasi-brittle materials with a random heterogeneous microstructure under various loading conditions for cohesive cracks. This was achieved by extracting only the active inelastic response occurring in the micro sample (rather than the whole responses in the micro sample as in standard homogenization schemes) to determine the equivalent homogenized macroscopic response.
Using Hill’s energetic equivalence condition in combination with the proposed failure zone averaging scheme, homogenization relations for both macroscopic adhesive and cohesive cracks were obtained for materials exhibiting diffusive damage. The proposed homogenization scheme can be considered as an aggregation of a micro localization band to a macro discontinuous crack in an energetically equivalent manner. The homogenization scheme was implemented in a standard strain-driven FE framework and successfully verified by three simple, proof-of-concept numerical examples. The proposed homogenization scheme is objective with respect to the micro model size apart being independent of macro and micro finite element discretizations. The method has been verified by comparing it with a direct numerical simulation. Numerical examples with more complexity will be given in the next chapter.
Chapter 6

Homogenization-based multiscale modelling of cracks: numerical aspects and applications

This chapter is a continuation of Chapter 5 regarding three aspects. Firstly, implementation details including a new way to compute the homogenized tangent, which is not available in literature, are presented. Secondly, an extension of the method to loading/unloading cases and a simple way to handle macroscopic snapback in a multiscale computation are given. Finally, some numerical examples including crack propagation are given to assess the performance of the method and suggestions to enhance the computation speed are given.

The remainder of the chapter is structured as follows. In Section 6.1, the finite element models utilized at the macro and micro scales are discussed together with the constitutive laws. Section 6.2 briefly presents the computational homogenization schemes for adhesive and cohesive cracks. The next section describes some implementational and computational aspects of the proposed multiscale crack modelling framework. Finally, some numerical examples are presented in Section 6.4 to demonstrate the performance of the method.

6.1 Macroscale and microscale models

In this section, the finite element models utilized at the macroscopic scale (called macroscale model) and the microscale (microscale model) are presented.

6.1.1 Macroscale model

Let us consider a two-dimensional solid \( \Omega_M \) shown in Figure 6.1 with its boundary denoted by \( \Gamma_M \). Prescribed tractions \( \bar{t} \) are imposed on the Neumann boundary \( \Gamma_M^c \subseteq \Gamma_M \) whereas prescribed displacements are imposed...
on the Dirichlet boundary $\Gamma^u_M \subseteq \Gamma_M$. The discontinuity surface $\Gamma^d_M$ is composed of cohesive cracks $\Gamma^\text{coh}_M$ and adhesive cracks $\Gamma^\text{adh}_M$. It is emphasized that although the material is heterogeneous, the macro solid is modelled as being homogeneous with effective properties coming from a heterogeneous micro model. Hereafter, subscripts $M$ and $m$ are used to indicate if a quantity belongs to the macro or micro scale, respectively.

The discrete equation for quasi-static equilibrium reads

$$f^\text{ext}_M = f^\text{int}_M \equiv f^\text{bulk}_M + f^\text{coh}_M$$

where $f^\text{ext}_M$ is the external force vector, $f^\text{int}_M$ is the internal force vector that consists of the bulk force vector $f^\text{bulk}_M$ and the cohesive force vector $f^\text{coh}_M$. They are given by

$$f^\text{ext}_M = \int_{\Omega_M} N^T b \, d\Omega + \int_{\Gamma^d_M} N^T t \, d\Gamma$$

$$f^\text{bulk}_M = \int_{\Omega_M} B^T \sigma \, d\Omega$$

$$f^\text{coh}_M = \int_{\Gamma^d_M} N^T t_{\text{M}} \, d\Gamma$$

where $\sigma_M$ is the macro Cauchy stress tensor, $b$ is the body force vector, $t$ is the applied traction and $t_{\text{M}}$ is the cohesive traction across the crack $\Gamma^d_M$. 

**Figure 6.1** A two-dimensional solid containing a cohesive crack and an adhesive crack. Note that $\Gamma^\text{coh}$ represents only the portion of the cohesive crack where $t_{\text{M}}$ is non-zero.
Some macro quantities like $b$ which do not appear at the microscale are written without subscript $M$. The strain-displacement matrix $B$ and the shape function matrix $N$, which depend on a specific finite element, are specified without subscript.

Partition of unity methods and zero thickness interface elements (see Chapter 2, Section 2.2.2) are utilized to model the cohesive and adhesive cracks, respectively. Note that only Heaviside enrichment is used, the cohesive cracks thus grow element-wise.

**Constitutive model**

The macroscopic bulk is assumed to be linear elastic with effective properties determined in a pre-processing step (before the multiscale simulation starts). That is

$$\sigma_M = D_0 \varepsilon_M$$

where $\varepsilon_M$ is the macro strain tensor and $D_0$ is the fourth-order tensor containing effective elastic moduli, which is computed by a conventional homogenization theory; we refer to Section 6.2.1 for the procedure.

The behavior of the adherents joined by the adhesive crack is independent of the microstructure of the adhesive crack. It can be modelled with any constitutive law. However, for the sake of simplicity, the adherents are assumed to be linear elastic.

The behavior of the macro cohesive and adhesive cracks is coming from the microscopic models. Thus, the macro cohesive law is generally given by

$$t_M = \Phi(\|u\|_M, \sigma_m)$$

where $\|u\|_M$ is the displacement jump across the macro crack and $\sigma_m$ is the micro stress tensor. Note that $\Phi$ is not explicitly constructed. Instead, $t_M$ is computed by averaging the micro stress tensor $\sigma_m$ of the sample associated to the integration point with the displacement jump $\|u\|_M$.

**Macroscale cohesive tangent**

The equilibrium equation (6.1) is solved in an incrementally iterative manner for the macroscale nodal displacements $u_M$. At Newton-Raphson iteration $i$ for a given load step, one has to solve the linear system $K_M^{-1} \Delta u'_M = \ldots$
Contributions to the macroscale tangent stiffness matrix $K_M$ include the bulk stiffness and cohesive stiffness matrices. The formula of the former is standard and hence not reported here. The latter is given by

$$K_M^{coh} = \int_{\Gamma_M} N^T T_M N d\Gamma$$

with $T_M$, the macroscale cohesive tangent, defined as

$$T_M = \frac{\partial \Phi}{\partial \| u \|_M}$$

### 6.1.2 Microscale model

The microscale model, shown in Figure 6.2, is a $w \times h$ rectangular domain $\Omega_m$ with external boundary $\Gamma_m$ where the heterogeneities are explicitly meshed. The geometry of the micro-model ($w$, $h$ and morphology of the microstructural constituents) depends on whether the macroscale crack to which this micro-model is associated is cohesive or adhesive, see Figure 6.1. Let us denote the characteristic length of the micro-constituents as $d$ (e.g., the mean diameter of the inclusions in a matrix/inclusion material) then the dimension of the microscale model must be large enough i.e., $w, h \gg d$ in order for the homogenized quantities to become independent of the microstructural randomness. When this condition is fulfilled, our proposed CH scheme is objective with respect to the micro-sample size.

The finite element model adopted at the microscale is the implicit gradient enhanced damage model described in Section 2.2.1, Chapter 2. The FE discrete equations, Equation (2.20), can be written in a general form as
\[
\mathbf{f}^\text{int}_m(\mathbf{u}_m) = \mathbf{f}^\text{ext}_m(\llbracket \mathbf{u} \rrbracket_M)
\]  \hspace{1cm} (6.9)

where \( \mathbf{u}_m \) represents the micro nodal unknowns vector. Note that \( \mathbf{u}_m \) contains both nodal displacements and nodal non-local equivalent strain degrees of freedom (dofs) \( \bar{\varepsilon}_\text{eq} \). In the proposed multiscale scheme, since the micro model is coupled to an integration point on the macro-crack, it is loaded by the displacement jump of this integration point. Thus, the microscopic external force vector depends on the macroscopic displacement jump.

### 6.2 Macro-Micro Coupling

In this section we elaborate on the macroscale/microscale coupling for cohesive cracks and adhesive cracks that was given in Chapter 5.

#### 6.2.1 Macro-micro coupling for cohesive cracks

![Schematic representation of the multiscale cohesive crack scheme.](image)

The problem that we are solving is that given a displacement jump \( \llbracket \mathbf{u} \rrbracket_M \) of an integration point on the macro crack, find the corresponding traction
Chapter 6 Multiscale crack modelling: numerical aspects and applications

\( t_M \). Borrowing ideas from conventional homogenization theories for bulk solids, this can be achieved by transforming \([u]_M\) to one micro model that is associated with this integration point, the micro BVP is then solved. The macro traction \( t_M \) is defined as a function of the micro stresses. Figure 6.3 presents the multiscale cohesive crack modelling framework. To reduce the implementation complexity and computer resources, in this work, it has been assumed that the RVEs for all integration points on a macro crack are identical.

The difficulty lies in how to define such a link which yields an objective macroscopic response with respect to the size of the micro-sample in the sense that when the micro-sample is large enough to be independent of the microstructural randomness, larger samples will lead to the same response. It has been shown in Chapters 4 and 5 that by extracting the micro response in the loading damaged domain (rather than in the entire micro domain as done in conventional homogenization theory), the homogenized macro response is independent of the micro model size.

The final homogenization relation is given by, see Chapter 5 for the derivation

\[
\begin{align*}
\mathbf{u}_R &= [w - l]C_0 \cdot t_M + [u]_M + \mathbf{u}_{\text{dam}} \\
&= [w - l]C_0 \cdot t_M + [u]_M + \mathbf{u}_{\text{dam}} \quad (6.10)
\end{align*}
\]

where \( \mathbf{u}_{\text{dam}} \) is computed upon micro softening occurs, \( C_0 \) is the projection of the compliance tensor \( D_0^{-1} \) on the macro crack plane and \( \mathbf{u}_R \) is the displacement of the right edge of the RVE, see Section 5.3 for details.

For macro load step \( n \) and macro Newton-Raphson iteration \( i \), at a Gauss point \( gp \) with \([u]_M\), the system of equations at the microscale is thus given by

\[
\begin{align*}
\mathbf{f}_m^{\text{int}}(\mathbf{u}_m) &= \mathbf{f}_m^{\text{ext}}([u]_M) \\
\mathbf{u}_R(\mathbf{u}_m) &= [w - l]C_0 \cdot t_M + [u]_M + \mathbf{u}_{\text{dam}} \quad (6.11a)
\end{align*}
\]

which is solved for the micro nodal unknowns \( \mathbf{u}_m \) and the macro traction \( t_M \). This system of equations is solved with an iterative scheme, refer to Chapter 5 for details. Box 6 gives a flowchart of the multiscale crack framework. Note that during step (A) in Box 6 the micro BVP must be solved \( m > 1 \) times. This is a crucial difference between the proposed method and the standard \( \text{FE}^2 \) method in which for step (A) the micro BVP is solved only one time.
Box 6 Flowchart of the multiscale cohesive crack framework.

1. For a macro load step \( n \), Newton-Raphson iteration \( i \) do
   a) Loop over crack segments to compute \( f_{\text{coh}}^M \)
      i. Loop over integration points on the crack segment
         - Get the macro jump \( [u]_M \)
         - Compute \( t_M \) and \( T_M \) with micro computations
            A. Solve the micro problem (step 4 Box 4 Chapter 5) \(^{(2)}\)
            B. Compute the macro traction \( t_M \) via Eq.(6.12a)
            C. Compute the macro tangent \( T_M \) via Eq.(6.12b)
      ii. End loop over integration points
   b) End loop over crack segments

2. Proceed to the next iteration

3. Upon convergence of load step \( n \), commit all micro internal variables.
   \(^{(1)}\) Computation of the bulk contribution \( f_{\text{bulk}}^M \) is done as in standard FEM.
   \(^{(2)}\) With micro state being reset to its previous converged values.

The macro traction and cohesive tangent matrix are (cf. Chapter 5) given by, respectively

\[
\begin{align*}
t_M &= \frac{1}{h} \sum_{I=1}^{n_b} f_{\text{int}}^{m,I} \\
T_M &= \frac{1}{h} M^T K_m^{*R} M
\end{align*}
\]  

(6.12a)  

(6.12b)

where \( n_b \) is the number of nodes on the right edge of the micro sample where the boundary conditions (BCs) are applied and the \( 2n_b \times 2 \) matrix \( M \) is given by

\[
M = \begin{bmatrix}
1 & 0 & 1 & 0 & \cdots & 1 & 0 \\
0 & 1 & 0 & 1 & \cdots & 0 & 1
\end{bmatrix}^T
\]  

(6.13)
and $K_{m}^{R}$ is the micro stiffness matrix associated with the right edge displacement dofs.

**Crack initiation/propagation criterion**

Following [194] the initiation/propagation criterion and the growth direction for the macro cohesive crack is purely macroscopic i.e., the macro crack propagates on the basis of the macro stress field. It is emphasized that microstructural effects influence the macro crack initiation because the macro stress field is computed from the effective properties, see Equation (6.5).

We utilize the maximum principal stress criterion as the crack initiation indicator and the non-local stresses, computed as a weighted average of macroscale stresses at the crack tip, to determine the crack direction (the crack is perpendicular to the maximum principal direction of the non-local stress tensor) [198]. It is noteworthy that other crack direction criteria such as the ones studied in [189] can be equally adopted. The criterion based on the non-local maximum principal stress is chosen simply due to its simplicity of implementation. Note that in [13, 15, 115] the macro crack direction has been computed using information from the micro model. In our opinion, this only makes sense when the microscopic length scale is of the same magnitude as the macroscopic length scale.

**Effective elasticity constants**

The effective elastic tangent moduli $D_{0}$ in Equation (6.5) can be determined using either analytical or computational homogenization. While the former is applicable to micro samples with simple morphology such as circular or elliptical inclusions, the latter can be used to any kind of microstructure and is therefore chosen to be used in this work. In order to compute $D_{0}$, we impose a macro strain vector $[\bar{\varepsilon}, 0, 0]$ to three corner nodes 1, 2 and 4 of the micro mesh, see Figure 6.4. The micro BVP is then solved with periodic boundary conditions which is simply a linear FE analysis. Upon convergence, Equation (2.62) is used to compute $D_{0}$.

**Tensile strength of the homogenized material**

Evaluation of the maximum stress criterion requires the tensile strength of the homogenized material. In the homogenization multiscale scheme, this value is defined as the ultimate load of the micro model $\sigma^{ult}_{m}$ subjected to a
horizontal tensile loading (for mode I failure studied in this work). In other words, in a pre-processing step, one micro model is loaded in tension along the horizontal direction and its ultimate load $\sigma_{\text{ult}}^m$ is computed as

$$\sigma_{\text{ult}}^m = \frac{1}{h} \sum_{l=1}^{n_h} f_{\text{int},l}^m (\tau)$$  \hspace{1cm} (6.14)

where $\tau$ denotes the instance at which the peak is attained.

**Micro model activation**

In a conventional homogenization approach for the bulk material and for an adhesive crack the micro-model is linked to a macroscale integration point *ab initio*. In contrast, the multiscale cohesive crack scheme presented in this Chapter uses a micro-model only when a new crack segment is initiated. Since the behavior of that new crack segment is determined only from the softening regime of the micro-model, this micro-model must be preloaded from an undeformed state to its peak. To this end, the micro-model is loaded, under load control, from zero up to $\bar{f} = \eta \sigma_{\text{ult}}^m h$ together with homogeneous BCs and periodic BCs as described in Section 6.2.3 with $\eta = 1 - \epsilon$, where $\epsilon$ is a small positive number, introduced to ensure convergence of this activation step. Furthermore, nodes on the right edge of the micro-model are forced to undergo the same displacement (see Figure 6.5). After being activated, the micro-model is loaded in displacement control, thus the force $\bar{f}$
and the aforementioned constraint are removed. This implies that the crack
initiation/propagation criterion reads $\sigma_{M}^{1} \geq \eta \sigma_{M}^{\text{ult}}$ where $\sigma_{M}^{1}$ denotes the
maximum macroscale principal stress. This load-control activation step is
achieved by dividing $\bar{f}$ into a number of sub-steps to ensure convergence.

Figure 6.5 Force control to activate the micro model
upon crack insertion. A force is applied to node 1
whereas other nodes on the right edge are forced to
have the same displacement as node 1.

Assumptions

The coupling between the macro-model and the micro-model is summa-
rized in Figure 6.6. Note that the pre-failure nonlinear (hardening) part of
the micro-model, indicated in Figure 6.6 by the darker region, is not cap-
tured by the macro-model. Therefore, an assumption was made that this
hardening part is negligible. As can also be seen, the homogenized cohesive
law is not strictly initially rigid but has a small hardening portion.

Remark 6.2.1. When the assumption on the negligibility of the microscopic
hardening part does not hold, modifications to the proposed scheme should
be made. One option is to compute the macroscale bulk constitutive model
on the fly as well. After crack nucleation, the macroscale bulk integration
points are no longer coupled to the micro-models but follow a linear elas-
tic law with effective properties evaluated at the crack nucleation moment.
The extension of the current multiscale scheme to relax the aforementioned
assumption is presented in the next chapter.

Principle of scale separation

This section discusses the issue of the principle of scale separation in the
cohesive crack multiscale model. Let us recall that there are two quantities
6.2 Macro-Micro Coupling

that are averaged in the proposed model - the bulk material surrounding the crack and the crack itself. The principle of scale separation applied for the bulk homogenization requires that the dimension of the micro-sample (for bulk homogenization) must be much smaller than the macroscopic length-scale so that the macroscale fields (stress or strain) are uniform over the micro-sample. For the crack homogenization, in order to satisfy the principle of scale separation, the micro-sample should be small enough compared to the macroscale fracture process zone (FPZ) so that the averaged quantities (e.g., $t_M$ or $\|u\|_M$) are constant over it. Since the FPZ is not known a priori, this condition is currently checked only a posteriori. One potential solution is that for cohesive integration points in the FPZ, if the principle of scale separation does not hold, micro-models with a smaller dimension are used. This kind of RVE-size adaptivity is a topic of future research.

6.2.2 Macro-micro coupling for adhesive cracks

Figure 6.7 presents the multiscale framework for an adhesive crack of thickness $t_{adh}$ that joints two adherents $\Omega_1^M$ and $\Omega_2^M$. The behavior of the adhesive crack is determined by means of a micro model that represents the microstructure inside the crack. The case in which the micro model width $w$ is equal to $t_{adh}$ is referred to as case I whereas the case in which $w < t_{adh}$ is denoted as case II.

![Figure 6.6](image.png)
Case I

When the micro-model width \( w \) equals \( t_{adh} \), and thus \( \mathbf{u}_R = [\mathbf{u}]_M \), the multiscale scheme becomes trivial. The macro-jump is directly imposed on the right edge of the RVE and the microscale BVP is solved. The macro-traction and the macroscale cohesive tangent are computed via Equations (6.12a) and (6.12b). This scheme was first presented in [110] for small strain problems and later in [73] for finite deformations and shares similarity with the one given in [92].

Case II

The homogenization equation that links the micro model to the macro model is given by (see Chapter 5, Section 5.3.2)

\[
\mathbf{u}_R = (w - t_{adh}) \mathbf{C}_0 \cdot \mathbf{t}_M + [\mathbf{u}]_M
\]

(6.15)

which provides the homogenization relation between microscale information and the macroscale cohesive law \((\mathbf{t}_M, [\mathbf{u}]_M)\). Comparing this expres-
sion with Equation (6.10) (for cohesive cracks) shows that Equation (6.15) was obtained from Equation (6.10) with \( l = t_{\text{adh}} \) (the compliance is now scaled with \( t_{\text{adh}} \)) and \( \dot{u}_{\text{dam}} = 0 \) (since the adhesive crack is present in the macro-model at the onset of the simulation).

The flowchart for the multiscale adhesive crack scheme is almost identical to the one for cohesive cracks given in Box 6. The only difference lies in step (A)- solving Equation (6.9) for the case I scheme and solving Equation (5.36) for the case II scheme.

### 6.2.3 Boundary conditions of micro model

Boundary conditions of the boundary nodes of the micro mesh are given by

\[
\begin{align*}
\text{periodic BCs} & : \quad u_T = u_B + u_2 - u_1 \\
\text{fixed BCs} & : \quad u_L = 0 \\
\text{prescribed BCs} & : \quad u_R = g(\|u\|_M)
\end{align*}
\]

(6.16)

refer to Figure 6.8 for notations. In the above, \( u \) indicates a vector containing the microscale displacement dofs. For the case I adhesive crack model, \( g(\|u\|_M) = \|u\|_M \) whereas for cohesive crack scheme and the case II adhesive scheme, refer to Chapter 5 for details. Note that these notations will be used in the sequel. This kind of BCs was first given in [110] and is referred to as hybrid BCs/semi-periodic BCs in [73].
6.3 Algorithmic aspects

In this section, various implementation details are presented. Note that basic implementation of a multilevel FEM can be found elsewhere for instance \cite{86}. The efficient solution of the micro nonlinear problem with periodic boundary conditions is first discussed. The extraction of the macro cohesive tangent matrix $T_M$ from the micro stiffness using the probing method is then presented. The advantage of this method is that it avoids the inversion of a large, sparse matrix and its explicit partition into sub-matrices. Treatment of arbitrary macro crack orientation i.e., the crack coordinate system is not aligned with the global coordinate system, is also given. To the best of the authors’ knowledge, works on homogenization have focused mainly on monotonic loading. We present here a discussion on computational homogenization for loading/unloading cases. Finally, resolving the snapback at the macroscopic scale with the dissipation-based arc-length control \cite{67} is presented.

6.3.1 Solution of the micro problem

In what follows, the master-slave method, used to solve the microscopic linear system with periodic constraints, is presented in details. It is emphasized that in \cite{73} the same topic has been presented. However, we present a somewhat different implementation and this section will be needed in subsequent presentation. In this section, the subscript $m$ is omitted for sake of clarity.

Let us first write the periodic BCs given in Section 6.2.3 in the following format

$$
\delta u_d = C \delta u_i \tag{6.17}
$$

where subscripts $d$ and $i$ denote dependent and independent degrees of freedom, see Figure 6.8.

The full micro displacement vector can be written in term of the independent displacement as

$$
\delta u = \begin{bmatrix} \delta u_i \\ \delta u_d \end{bmatrix} = \begin{bmatrix} I & C \end{bmatrix} \delta u_i \equiv T \delta u_i \tag{6.18}
$$
with \( I \) is a \([3n_i \times 3n_i]\) identity matrix (\( n_i \) is the number of independent nodes) and \( T \) is the so-called transformation matrix which is a rectangular matrix.

The microscopic linearized system is partitioned as

\[
\begin{bmatrix}
K_{ii} & K_{id} \\
K_{di} & K_{dd}
\end{bmatrix}
\begin{bmatrix}
\delta u_i \\
\delta u_d
\end{bmatrix} =
\begin{bmatrix}
r_i \\
r_d
\end{bmatrix}
\tag{6.19}
\]

By substituting Equation (6.18) into the above and pre-multiplying both sides with \( T^T \) we obtain

\[
\begin{bmatrix}
I & C^T
\end{bmatrix}
\begin{bmatrix}
K_{ii} & K_{id} \\
K_{di} & K_{dd}
\end{bmatrix}
\begin{bmatrix}
I & C
\end{bmatrix}
\begin{bmatrix}
\delta u_i \\
\delta u_d
\end{bmatrix} =
\begin{bmatrix}
I & C^T
\end{bmatrix}
\begin{bmatrix}
r_i \\
r_d
\end{bmatrix}
\tag{6.20}
\]

which yields the sought-for reduced system

\[
K^* \delta u_i = r^*
\tag{6.21}
\]

with \( K^* \), a \([3n_i \times 3n_i]\) matrix and \( r^* \), a \([3n_i \times 1]\) vector given by

\[
K^* = T^T K T
\]
\[
r^* = T^T r
\tag{6.22}
\]

Usually Equation (6.21) is solved for the independent displacement increments first and then the dependent displacement increments are computed via Equation (6.17), see also [73, 86]. Here, we prefer solution methods that do not alter the dimension of the stiffness matrix. This has several advantages. First, there is no need to keep track of which dof corresponds to which unknown in the linear solver. Second, there is no need to store a new, constrained matrix if the linear system is solved with an iterative solver. In this case we just keep the original matrix, and apply the matrix \( T \) in each matrix-vector multiplication. A third advantage is that in parallel computations each processor can setup and apply constraints without having to modify the communication data structures in the linear solver. Precisely, the following system is solved instead of Equation (6.21)
In words, the matrix $K^*$ has been augmented with the trivial equation $I\delta u_d = \delta u_d$ so that $\overline{K}_m$ is of the same dimension as $K_m$.

**Remark 6.3.1.** The motivation for premultiplying Equation (6.19) with $T^T$ in order to obtain Equation (6.20) is as follows. Matrix $T$ essentially encodes the relationship between the independent dofs and all dofs, including the dependent dofs. This means that matrix $T^T K T$ can be viewed as the projection of matrix $K$ on a vector space spanned by the independent dofs. In other words, the full system of equations is projected on the vector space spanned by the independent dofs and is then solved for the resulting, smaller system of equations.

### 6.3.2 Probing method to compute the macro tangent

Equation (6.23) can be written in the following format at the converged state of the microscale BVP

$$
\begin{bmatrix}
T^T K_m T & 0 \\
0 & I \\
\end{bmatrix}
\begin{bmatrix}
\delta u_l \\
\delta u_d \\
\end{bmatrix} =
\begin{bmatrix}
r^* \\
\delta u_d \\
\end{bmatrix} 
(6.23)
$$

with $b$ denoting dofs associated with nodes on the right edge and $a$ are the dofs of the remaining nodes excluding top nodes, see Figure 6.8. The above allows the following condensation

$$
K_m^{+,bb} \delta u_m^b = \delta f_b 
(6.25)
$$

with

$$
K_m^{+,bb} = \overline{K}_m^{bb} - \overline{K}_m^{ba}(\overline{K}_m^{aa})^{-1}\overline{K}_m^{ab} 
(6.26)
$$
This $3n_b \times 3n_b$ matrix can be filtered to get $K^{+,R}_m$, a $2n_b \times 2n_b$ matrix, as

$$K^{+,R}_m = A^T K^{+,bb}_m A$$  \hspace{1cm} (6.27)

where $A$ is a $3n_b \times 2n_b$ boolean matrix.

Substituting Equation (6.26) into Equation (6.12b) yields

$$T_M = \frac{1}{h} M^T A^T [K^{bb}_m - K^{ba}_m (K^{aa}_m)^{-1} K^{ab}_m] A M$$  \hspace{1cm} (6.28)

For materials with complex multi-phase microstructures, the micro stiffness matrix $K_m$ could be a very large, sparse matrix of which inversion and partition operations are obviously inefficient. In order to avoid them, we use the so-called probing technique that is a very simple technique to construct a matrix, here $T_M$, from a series of matrix-vector products. This matrix is built in a columnwise manner. The first column of $T_M$ is computed by multiplying the RHS of Equation (6.28) with $e_1 = [1 \ 0]^T$

$$T^1_M = \frac{1}{h} M^T A^T [K^{bb}_m f - K^{ba}_m (K^{aa}_m)^{-1} K^{ab}_m f], \quad f = A M e_1$$  \hspace{1cm} (6.29)

In order to compute $K^{bb}_m f$ and $K^{ab}_m f$, it suffices to do the following matrix-vector multiplication

$$\begin{bmatrix} K^{aa}_m & K^{ab}_m \\ K^{ba}_m & K^{bb}_m \end{bmatrix} \begin{bmatrix} 0 \\ f \end{bmatrix} = \begin{bmatrix} K^{ab}_m f \\ K^{bb}_m f \end{bmatrix} \equiv \begin{bmatrix} g \\ h \end{bmatrix}$$  \hspace{1cm} (6.30)

The first column of $T_M$ is then given by

$$T^1_M = \frac{1}{h} M^T A^T [h - K^{ba}_m (K^{aa}_m)^{-1} g]$$  \hspace{1cm} (6.31)

To compute $(K^{aa}_m)^{-1} g$, it suffices to solve the following linear system

$$\begin{bmatrix} K^{aa}_m & K^{ab}_m \\ K^{ba}_m & K^{bb}_m \end{bmatrix} \begin{bmatrix} u \\ 0 \end{bmatrix} = \begin{bmatrix} g \\ 0 \end{bmatrix}$$  \hspace{1cm} (6.32)
Finally, to compute $K_{m}^{ba}(K_{m}^{aa})^{-1}g = K_{m}^{ha}u$, the following matrix-vector multiplication is used

$$
\begin{bmatrix}
K_{m}^{aa} & K_{m}^{ab} \\
K_{m}^{ba} & K_{m}^{bb}
\end{bmatrix}
\begin{bmatrix}
u \\
0
\end{bmatrix}
= 
\begin{bmatrix}
K_{m}^{aa}u \\
K_{m}^{ba}u
\end{bmatrix}
\equiv 
\begin{bmatrix}
m \\
l
\end{bmatrix}
$$

(6.33)

To summarize, the first column of the consistent tangent moduli is given by

$$
T_{M}^{l} = \frac{1}{h}M^{T}A^{T}(h - I)
$$

(6.34)

which consists of the solution of a linear system Equation (6.32) and two matrix-vector multiplications.

In the same manner, the second column of $T_{M}$ is computed with $e_{2} = [0 \, 1]^{T}$. As demonstrated, the procedure we follow does not directly compute any inverted matrix. Furthermore, all the calculations involve only the total RVE matrix. No explicit sub-matrix is needed. For ease of implementation, the procedure is given in Box 7.

**Remark 6.3.2.** It is emphasized that in [182] authors have proposed a perturbation method to compute the macroscopic tangent in a multilevel finite element setting as an alternative to the standard condensation procedure. Their reasoning was to avoid the use of extensive computer memory required to store the microscopic sub-matrices. We have presented an implementation in which the standard condensation is utilized that does not need to allocate any new sub-matrix.

### 6.3.3 Handling arbitrary macro crack direction

The discussion so far applies for the case in which the crack normal is parallel to the lower edge of the RVE. If this is not the case as shown in Figure 6.9a, there are two options. As the first option, the geometry of the micro-model is rotated in order to align it with the macro-crack, see Figure 6.9b. According to the second option (adopted in this work), applicable to materials with a microstructure having an isotropic geometry (e.g., random microstructure as the target material in this work), the orientation of the micro-model is fixed (Figure 6.9c) and we proceed as follows. The global macro-jump vector is transformed to the local coordinate system associated with a point on the crack surface by
**Box 7** Computation of the macro tangent with the probing method

1. Assembling the micro stiffness $K_m$
2. Constructing the modified matrix $\overline{K}_m$ using Eq.(6.23).
3. Initialize $3n \times 1$ vectors $d = 0$ and $f_1 = 0$
4. For $i = 1, 2$, do
   a) Compute $f = Me_i$
   b) Set $d[b] = f$
   c) Compute $\text{rhs} = \overline{K}_m d$, then $g = \text{rhs}[a]$, $h = \text{rhs}[b]$
   d) Solve the linear system $\overline{K}_m u = f_1$ with $f_1[a] = g$ *
   e) Compute $\text{rhs} = \overline{K}_m u$, then $m = \text{rhs}[a]$, $l = \text{rhs}[b]$
   f) Compute column $i$ as $T^i_M = \frac{1}{h} M^T (h - 1)$
5. End for

* With homogeneous boundary conditions $u[b] = 0.$

**Figure 6.9** Arbitrary macro crack orientation (a), rotated RVE geometry (b) and (c)-fixed RVE geometry (applicable to microstructure having isotropic geometry).

\[
[u]_{ns} = Q[u]_M
\]  

(6.35)

This local jump vector is then used as boundary conditions imposed on the RVE’s boundaries. The first component of $[u]_{ns}$ is used as boundary condi-
tions along $x^1_m$ direction and the second one along $x^2_m$ direction. After solving the RVE problem, one obtains the macro traction and tangent in the local coordinate system, $t_{ns}$ and $T_{ns}$. Using Equation (6.12a) and Equation (6.12b), respectively, they are transformed back to the global coordinate system as follows

$$t_M = Qt_{ns} \quad T_M = QT_{ns}Q$$

(6.36)

with $Q$ being the orthogonal transformation matrix, see [5]. Figure 6.9 illustrates the idea.

It should be emphasized that the above approach works for materials with microstructure having isotropic geometry e.g., random microstructure as the target materials in this work. For columnar materials like masonry, one has to rotate the geometry of the micro model.

**Remark 6.3.3.** Note that the option described in Figure 6.9b is general i.e., it can be applied to any material whereas the option given in Figure 6.9c saves computational efforts for materials with isotropic geometry. Furthermore, it is emphasized that the proposed approach would not work for non-proportional loadings. For example, an initial loading causes damage in the micro-sample, then unloading occurs, and the load direction is changed, subsequently causing the micro-sample to be further damaged. Because of the first damaging phase the micro-sample becomes anisotropic thus violating the assumption of isotropy of the micro-sample upon which the proposed approach has been developed i.e., the proposed algorithm would be invalid.

As an example to illustrate the idea, let us consider the problem shown in Figure 6.10 which consists of two homogeneous elastic adherents joined together by a voided damageable adhesive layer. The sample is fixed in the vertical direction at the bottom edge and in the horizontal direction on the left and right edges. These BCs ensure that a homogeneous state of deformation is obtained for all integration points on the adhesive crack. A uniform vertical displacement is imposed on the top edge. A plane stress condition is assumed. Finite element meshes of the Direct Numerical Simulation (DNS) model and the multiscale model (case I model) are given in Figure 6.11. Figure 6.12 gives the comparison of the load-displacement curves of the DNS and multiscale model. We attribute the small discrepancy between the two solutions to the mismatch of geometries at the boundaries of the adhesive.
6.3 Algorithmic aspects

**Figure 6.10** Inclined material layer having a periodic voided microstructure. Unit of length is mm.

**Figure 6.11** Inclined material layer: DNS mesh and multiscale meshes. The thick line denotes the interface elements.

layer used in DNS and multiscale simulations, see Figure 6.13. Damage patterns in the DNS and in the RVEs are shown in Figure 6.14.

### 6.3.4 Loading/unloading treatment

**Adhesive crack-case I** Let us first consider Case I (micro sample width \( w \) equals \( t_{adh} \)). Since \( \mathbf{u}_R = \mathbb{[u]}_M \), unloading is handled naturally i.e., macro unloading follows micro unloading. Therefore, no further work is needed.

\[
\begin{align*}
E &= 25000 \text{ MPa} \\
\nu &= 0.2 \\
\kappa_l &= 3 \times 10^{-05} \\
\gamma &= 0.999 \\
\beta &= 5000 \\
c &= 3.5 \text{ mm}^2
\end{align*}
\]
Figure 6.12 Inclined material layer: comparison of load-displacement curves between DNS and multiscale analysis.

![Graph showing load-displacement curves for DNS and FE2.]

**Figure 6.12** Inclined material layer: comparison of load-displacement curves between DNS and multiscale analysis.

![Diagram showing geometry mismatch in DNS and multiscale (case I) models.]

**Figure 6.13** Inclined material layer: Geometry mismatch in DNS and multiscale (case I) models.

![Diagram showing damage pattern in DNS and RVEs.]

**Figure 6.14** Damage pattern in the DNS (left) and in RVEs associated with interface elements (right).
6.3 Algorithmic aspects

**Adhesive crack-case II/cohesive crack** For Case II, we have $\mathbf{u}_R \neq [\mathbf{u}]_M$ and for cohesive cracks, the failure zone averaging scheme fails when unloading occurs (because the active damaged domain $\Omega_d$ is empty). For these reasons, loading/unloading is treated with a history variable being the maximum opening displacement ever reached $[\mathbf{u}]_M^{\text{max}}$. Assuming secant unloading, the macro traction is then defined as

$$t_M = \frac{t_M^{\text{max}}}{[\mathbf{u}]_M^{\text{max}}} [\mathbf{u}]_M$$  \hspace{1cm} (6.37)

since $t_M^{\text{max}}$ cannot be analytically computed from $[\mathbf{u}]_M^{\text{max}}$ due to the lack of a phenomenological cohesive law, it is computed from the micro model corresponding to the state right before unloading occurs. Note that during macro unloading, the micro model is not loaded and thus no micro BVP is needed to be solved.

![Figure 6.15](image)

**Figure 6.15** A simple problem (all units in mm) with a vertical material layer having thickness of 40 mm. The layer is made of a periodic voided microstructure. Three RVEs (voids with a radius of 5) shown in the right are investigated.

As an example for handling loading/unloading in a multiscale simulation, we consider a simple test given in Figure 6.15 which consists of two adherents joined by an adhesive layer of 40 mm thickness. The specimen is loaded under displacement control. When the prescribed displacement $\bar{u}$ equals 0.4 mm, the sample is completely unloaded and then reloaded until final failure of the sample. A plane stress condition is assumed. Material properties of the micro model can be found in Figure 6.10 except for the softening slope $\beta$ which equals 3000.
The load-displacement curves shown in Figure 6.16 demonstrate, for both case I (micro models 40 × 40 and 40 × 20) and case II (micro model 20 × 20) schemes, the objectivity of the macro response with respect to the adopted micro model for loading/unloading conditions.

6.3.5 Macroscale snapback with dissipation based arc-length control

Tracing equilibrium paths with snap through and snapback points has been traditionally undertaken by means of path-following methods (also known as arc-length methods), see for instance [38, 51]. A very elegant method has been recently introduced in [67, 193] to trace complex equilibrium paths, refer to [191] for application examples. In this section, we present a preliminary study on resolving macroscopic snapback in a multiscale setting. Note that for the particular material model we are using at the microscale, no microscale snapback has occurred. If this is about to happen, a solution reported in [107] can be used. To the best of our knowledge, no multiscale simulation which involves both macroscopic and microscopic snapback has been reported in literature.

According to the dissipation-based arc-length method [67, 193], the macro system of equations is given by

\[
\begin{align*}
\bar{f}_{\text{int}}(\mathbf{u}_M) &= \lambda \bar{\mathbf{f}} \\
\phi(\lambda, \mathbf{u}_M) &= 0
\end{align*}
\]

(6.38)

where \( \bar{\mathbf{f}} \) is a unit force vector, \( \lambda \) is the so-called load factor and \( \phi \) is a con-
contains an equation that, for a given load step, defines $\lambda$ in such a manner that a predefined amount of energy $\Delta \tau$ is released. For details, refer to [67]. Contrary to other arc-length methods, this equation is defined in terms of global quantities and hence there is no need to keep track of areas where localized nonlinearity is taking place. Usually, $\Delta \tau$ is bounded by

$$\tau_{\text{min}} \leq \Delta \tau \leq \tau_{\text{max}}$$

(6.39)

where $\tau_{\text{min}}$ is used to save unnecessarily small load increments and $\tau_{\text{max}}$ is used to avoid too large increments. Additionally, in a FE$^2$ setting, $\Delta \tau$ must be sufficiently small so that all micro models converge. Since a universal rule for $\Delta \tau$ that ensures convergence of the macro model and all micro models is missing, when a micro model diverges, the corresponding macro load step is resolved with smaller $\Delta \tau$. Another option is to use the sub-stepping scheme presented in [171] to resolve the diverged micro model.

Figure 6.17 describes the considered problem that shows macroscopic snapback behavior. The macro-mesh is composed of two four-noded quadrilateral (Q4) elements with one interface element in between.

Figure 6.17 A simple test with macro-snapback behaviour. The voids have a radius of 5. Unit of length is mm. The macro-mesh is composed of two Q4 elements with one interface element in between.

Figure 6.17 describes the considered problem that shows macroscopic snapback behavior. The macro-mesh is simply composed of two four-noded quadrilateral (Q4) elements with one interface element in between of which behavior is coming from two micro-samples, the $40 \times 20$ mm$^2$ one for the case I scheme and the $20 \times 20$ mm$^2$ one for the case II scheme. A plane stress condition is assumed. The macroscale load-displacement curves obtained with two different values of $\Delta \tau_{\text{min}}$ are given in Figure 6.18.
Chapter 6 Multiscale crack modelling: numerical aspects and applications

Figure 6.18 Handling macroscopic snapback with a dissipation-based arc-length control in the multiscale adhesive crack scheme.

(a) $\Delta \tau_{\text{min}} = 0.02 \text{ N mm, case I}$  (b) $\Delta \tau_{\text{min}} = 1 \times 10^{-4} \text{ N mm, case I}$

Figure 6.19 A simple problem with one cohesive crack that shows macroscopic snapback. All units are in mm.
For cohesive cracks, let us consider the problem depicted in Figure 6.19. Material parameters for the micro-model are given in Figure 6.17 except for $\beta$ which is set to 6000. A plane stress condition is assumed. The load-displacement curve is given in Figure 6.20. A value $\Delta \tau_{\min} = 1 \times 10^{-3} \text{ N mm}$ was used.

We have shown that the dissipation-based arc-length control method presented in [67] can be seamlessly adopted in the proposed multiscale crack modelling framework. It should be mentioned that secant unloading is the critical assumption for allowing the dissipation-based arc-length control to work.

### 6.4 Numerical examples

In this section, four numerical examples are given to demonstrate the performance of the proposed multiscale method. In the first example (Section 6.4.1), a simple macro-sample in uni-axial tension is analyzed. The microstructure is, however, a complex random multi-phase material. The aim of this example is to verify the objectivity of the method with respect to the micro-model size. The convergence property of the presented method is investigated in the second example (Section 6.4.2). The wedge splitting test, which is analyzed in the third example (Section 6.4.3), compares the multiscale method with a DNS. Finally, failure of a single edge notched beam (SEN) which involves the propagation of a curved crack is given in the final
example (Section 6.4.4). The finite element meshes used in this section have been generated using Gmsh [54] except the concrete micro-samples in the first and fourth example that have been created using SPACE [176].

6.4.1 RVE’s existence test

In order to verify the objectivity of the multiscale solution with respect to the micro-model size, the macro sample as shown in the top of Figure 6.21 is analyzed.

![Geometry, finite element discretization of the macro-model (left) and micro-samples (right) for the RVE’s existence test. All units are in mm.](image)

Upon satisfaction of the failure criterion, \( \sigma_M^I \geq 0.97 \sigma_m^{ult} \), a vertical crack is initiated in the middle element (only one crack is allowed in this example). The behavior of this crack comes from FE computations realized on
two micro-samples made of a three-phase material (aggregate, matrix and ITZ) of which material parameters can be found in Table 6.1. Both samples correspond to a 45% volume fraction of aggregates (of which radius varies from 2.5 mm to 5.0 mm). The width of the ITZ is 0.25 mm. The microscale FE meshes consist of 10 052 and 18 208 three-noded triangular elements (T3 elements) for the 15 × 15 mm$^2$ and the 20 × 20 mm$^2$ sample, respectively. A plane strain condition is assumed for the micro-models. The effective elastic moduli $D_0$ computed using the continuous CH approach described in Section 2.4 are

<table>
<thead>
<tr>
<th></th>
<th>Matrix</th>
<th>Aggregate</th>
<th>ITZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [N/mm$^2$]</td>
<td>25 000</td>
<td>30 000</td>
<td>20 000</td>
</tr>
<tr>
<td>$\nu$ [-]</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$\kappa_1$ [-]</td>
<td>5e-06</td>
<td>0.5</td>
<td>3e-06</td>
</tr>
<tr>
<td>$\gamma$ [-]</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
</tr>
<tr>
<td>$\beta$ [-]</td>
<td>1500</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>$c$ mm$^2$</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Table 6.1 Material parameters of different phases of the random heterogeneous material.

$$D_{0}^{15} = \begin{bmatrix} 29903.0 & 7485.55 & -1.15865 \\ 7485.55 & 29905.9 & 0.919313 \\ -1.15865 & 0.919313 & 11213.6 \end{bmatrix}$$

for micro-sample 15 × 15 mm$^2$ and

$$D_{0}^{20} = \begin{bmatrix} 29804.3 & 7456.68 & 0.135379 \\ 7456.68 & 29812.1 & 0.0845691 \\ 0.135379 & 0.0845691 & 11173.7 \end{bmatrix}$$

for micro-sample 20 × 20 mm$^2$, respectively.

The objectivity of the macroscale solution with respect to the micro-model size can be judged from Figure 6.22 which shows the macroscale load-displacement curves obtained with two micro-samples. Tests have shown
that micro-samples smaller than $15 \times 15 \text{mm}^2$ yield a different macroscale solution since these micro-samples are not large enough, see also Chapter 4. The homogenized cohesive laws are also given in this figure. Note that since the crack was inserted slightly before the ultimate load of the micro-model, the homogenized cohesive laws are not initially rigid as conventional cohesive laws.

![Figure 6.22](image-url)  
Figure 6.22 RVE’s existence test: objective macroscopic load-displacement diagrams obtained with various microstructures (left) and homogenized traction-opening laws (right).

**Remark 6.4.1.** The number of load increments required to solve the macroscopic BVP from the moment of crack nucleation until final failure is denoted as $n$. Each macroscale load increment is done with an averaged number of $m$ Newton-Raphson iterations. For one macroscale Newton-Raphson iteration one has to solve $2p$ micro-BVPs (in this example there is only one crack segment with 2 integration points). Therefore, the total number of micro-BVPs is $n \times m \times 2p$. Considering that $n = 60$, $m = 4$ and $p = 2$, then for this simple example one has to solve 480 micro-BVPs of dimension 30,156 dofs (for the $15 \times 15 \text{mm}^2$ sample). Needless to say, advanced techniques that are capable of reducing the computational cost of the proposed multiscale scheme are welcome. One promising avenue is model order reduction methods applied to the microscale boundary value problem. Basically, the solution to the microscale BVP is searched in a coarse space that is spanned by a reduced order basis. The proper orthogonal decomposition (POD) can be used to define this reduced order basis from representative solutions (usually called snapshots). Snapshots are solutions of the standard (full order) microscale BVP subject to different BCs. Basic ideas have been set in [84, 127].
6.4 Numerical examples

6.4.2 Convergence properties of the multiscale scheme

This example aims to obtain insights in the convergence rate of the three multiscale schemes presented before: adhesive crack scheme (case I and case II) and cohesive crack scheme. The use of a consistent tangent matrix at the microscale yields an optimal quadratic convergence rate for the microscale problem. Hence convergence properties of the microscale problem are standard and therefore not reported. Rather, we focus on the convergence performance of the Newton-Raphson iterative method used at the macroscale and on the convergence behaviour of the iterative scheme used to solve Equations (6.11) and (5.39).

For adhesive cracks, let us reconsider the problem given in Figure 6.15, Section 6.3.4. Material properties of the micro-model can be found in Figure 6.10. The sample is loaded under displacement control with a constant step $\Delta u = 0.0001$ mm. For the case I scheme (micro-model is $40 \times 20$ mm$^2$), the load-displacement diagram and the number of Newton-Raphson (NR) iterations required for each macroscale load increment is given in Figure 6.23. A quadratic convergence rate can be observed from Table 6.2. Note that load step 31 is a difficult one since the slope is almost vertical. That explains why 6 NR iterations were required for this step.

The residual $r$ given by

$$ r = \frac{\left| f_{\text{ext}}^M - f_{\text{int}}^M \right|}{\left| f_{\text{ext}}^M - f_{\text{int}}^M \right|} \tag{6.40} $$

represents the standard scaled residual between the current iteration $i$ and

![Figure 6.23](image-url) Adhesive scheme-case I: Load-displacement curve (left) and the Newton-Raphson iterations per macroscale load step (right).
the first iteration. In the above, \( || \cdot || \) is the L_2 norm.

<table>
<thead>
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<th>Step no.</th>
<th>Iteration no.</th>
<th>Residual r</th>
</tr>
</thead>
<tbody>
<tr>
<td>31</td>
<td>1</td>
<td>4.6334e-02</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.4752e-02</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2.5577e-02</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>3.5018e-03</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>1.1404e-04</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>1.3562e-07</td>
</tr>
<tr>
<td>36</td>
<td>1</td>
<td>3.3328e-02</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.7055e-04</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4.3285e-09</td>
</tr>
</tbody>
</table>

Table 6.2: Adhesive scheme-case I: performance of the macroscale NR scheme.

We now turn our attention to the adhesive crack-case II scheme. In this case, the \( 20 \times 20 \text{ mm}^2 \) micro-model is used. Figure 6.24 shows the load-displacement diagram and the number of NR iterations required for each macroscale load increment. We attribute the need of a large number of NR iterations (19) for macroscale load step 31 to two reasons. The first one is the almost vertical slope of the load-displacement curve at that point. The second reason is that step 31 is the transition step from a hardening regime to a softening regime. Let us recall that we use two different schemes for the hardening and the softening parts, Section 5.4.2. By using a less steep softening slope \( \beta = 3000 \) (so far \( \beta = 5000 \) was used), the maximum number of NR iterations reduces to 4 as can be seen in Figure 6.25.

The bottom part of Figure 6.24 gives the number of micro-BVPs that are solved for every macroscale NR iterations. As can be seen, far from the peak, the micro-BVP is solved only one time per macroscale NR iteration which is similar to standard FE² methods.

For the cohesive crack homogenization scheme, the problem given in Figure 6.19 is considered again. Material properties of the micro-model can be found in Figure 6.10 except for \( \beta \) which is set to 1000 to have a smooth macroscale equilibrium path. Figure 6.26 shows the load-displacement di-
6.4 Numerical examples

Figure 6.24 Adhesive scheme-case II: load-displacement curve (top left), Newton-Raphson iterations per macroscale step (top right) and number of micro-BVPs for every macroscale Newton-Raphson iterations (bottom).

Figure 6.25 Adhesive scheme-case II, smooth response with $\beta = 3000$: load-displacement curve (left), Newton-Raphson iterations per macroscale step (right).
Table 6.3 Cohesive crack scheme: performance of the macroscale Newton-Raphson method.

<table>
<thead>
<tr>
<th>Step no.</th>
<th>Iteration no.</th>
<th>Residual $r$</th>
</tr>
</thead>
<tbody>
<tr>
<td>17</td>
<td>1</td>
<td>1.0189e-02</td>
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<td>2</td>
<td>6.9791e-04</td>
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<td>1.2804e-04</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>3.3568e-08</td>
</tr>
</tbody>
</table>

Figure 6.26 Cohesive crack scheme: load-displacement curve (top left), Newton-Raphson iterations per macroscale step (top right) and number of micro-BVPs for every macroscale Newton-Raphson iterations (bottom).

agram and the number of NR iterations required for each macroscale load increment. Three NR iterations are needed for macroscale steps round the
peak. The reduction in residuals for two macroscale load increments around the peak is tabulated in Table 6.3. The bottom part of Figure 6.26 gives the number of micro-BVPs that are solved for every macroscale NR iterations. Far from the peak, the micro-BVP is solved only one time per macroscale NR iteration which is similar to standard FE methods.

6.4.3 Wedge splitting test

The wedge splitting test, given in Figure 6.27, is studied in this example. The sample is made of a matrix-fiber material (with a weak transition zone, ITZ, to model matrix-fiber interface debonding). In order to reduce the computational cost, the microstructure is only explicitly resolved in the region in front of the notch where the crack is expected to develop and grow. The rest (shaded region) is modelled as homogeneously linear elastic with effective properties (the Young’s modulus is 12 647.66 N/mm² and the Poisson’s ratio is 0.2). Material in the red region follows the isotropic non-local damage model described in Chapter 2 with material parameters being given in Table 6.4. The analysis is performed under a plane stress state with displacement control. This example is specially designed in order to make a comparison of the proposed multiscale model with a DNS. A simple microstructure is taken and a single localization band is promoted.

The FE discretization of the DNS model, shown in Figure 6.28, consists

![Figure 6.27 Wedge splitting test: geometry (units in mm) and boundary conditions.](image)
of 25,368 three-noded triangular elements and 12,778 nodes (36,366 dofs). Finite element meshes of the macro-model and micro-model in a multiscale simulation are given in Figure 6.29. When $\sigma_M^t \geq 0.999\sigma_M^{ult}$, the macro-crack initiates/propagates. In this example, due to symmetry, the crack direction at the macroscale is forced to be horizontal.

$$\begin{array}{ccc} 
E & 25,000 & 30,000 & 20,000 \\
\nu & 0.2 & 0.2 & 0.2 \\
\kappa_1 & 5\times10^{-5} & 0.5 & 3\times10^{-5} \\
\gamma & 0.999 & 0.999 & 0.999 \\
\beta & 100 & 100 & 100 \\
c & 0.005 & 0.005 & 0.005 
\end{array}$$

**Table 6.4** Material parameters of different phases of the fiber-reinforced composite.

Evolution of damage in the DNS and evolution of the macro-crack in the $\text{FE}^2$ model is shown in Figures 6.30 and 6.31. An observation was made from Figure 6.30 that the macro-crack in the multiscale model runs slightly behind the localization band in the DNS. We attribute this to two facts namely (i) the macroscopic load increments are larger for the $\text{FE}^2$ simulation than for the DNS to reduce the computation time and (ii) the difference in the failure criterion. In DNS, a strain-based damage initiation criterion was used and in $\text{FE}^2$ a stress-based crack initiation criterion was adopted. It can be observed from Figure 6.32 that boundary effects are still not properly handled in the multiscale model. A remedy is to apply periodic BCs only for interior RVEs (e.g., RVEs far from the boundaries) and better tailored BCs for boundary RVEs. This boundary effect was also noted in [15, 48]. This is a topic of further research.

Comparison of the load-displacement curves of the DNS and multiscale model (denoted by $\text{FE}^2$) is depicted in Figure 6.33. The peak load obtained with the DNS is 48.70 N while the peak load obtained with the multiscale model is 48.36 N. The curve associated with the multiscale model is not smooth due to two facts (i) the macroscopic load increment steps are large (to reduce the computation time) and (ii) the mesh of the macro-model is coarse (keep in mind that in our PUM implementation, the crack grows
6.4 Numerical examples

Figure 6.28 Wedge splitting test: FE mesh of the DNS model (25368 three-noded triangular elements). Elements of the matrix phase in the upper part (red color) are not allowed to be damaged.

Figure 6.29 Wedge splitting test: FE meshes of the multiscale model. Macro-mesh consists of 1426 three-noded triangular elements whereas micro-mesh composed of 4092 T3 elements. A crack is initiated at point A and grows horizontally to the right edge. In the RVE, elements of the matrix phase in the right part (red color) are not allowed to be damaged. Since the macro-crack direction is horizontal whereas the micro localization band is vertical, the algorithm given in Section 6.3.3 is used.
element-wise). It is emphasized that in order to make a fair comparison between the DNS and the FE\textsuperscript{2}, we have, in the DNS, prevented damage from starting in the corners, see Figure 6.28.

Concerning the computational cost, the DNS time was 14 hours while the FE\textsuperscript{2} time was only 4 hours i.e., 3 times faster.

### 6.4.4 Single edge notched beam

As an example of a curved propagating crack analysis in the presented multiscale cohesive crack framework, let us consider the single edge notched beam given in Figure 6.34. This problem has been studied experimentally in [159] and numerically in a monoscale setting by, for instance, [198] and in a multiscale setting by [13, 194]. In [194], the authors have studied the influence of the microstructure on the macroscale ultimate load. For this reason, the post-peak response has not been reported. Here, we focus on the issue of robustness of the proposed multiscale scheme. The aim is to show that a complete multiscale analysis for curved crack propagation can be achieved. No comparison against a DNS is therefore performed. Hence, the size of the
6.4 Numerical examples

Figure 6.31 Wedge splitting test: damage pattern in the DNS model (top) at the moment that the localization band approaches the right edge of the specimen and crack path with damaging RVEs in the FE$^2$ model (bottom). The contour plot for the macro sample of the multi-scale analysis shows the displacement field in the vertical direction.

Figure 6.32 Boundary effects: periodic BCs are not suitable for boundary RVEs.
Chapter 6 Multiscale crack modelling: numerical aspects and applications

Figure 6.33 Wedge splitting test: comparison of load-displacement curves between the DNS and the multiscale cohesive crack scheme.

The micro model is chosen without considering the principle of scale separation (as can be seen in Figure 6.35, the micro model is not small compared to the macro model).

Figure 6.34 Single edge notched beam (SEN): geometry (all units are in mm), boundary conditions. The depth of the beam is 100 mm. The crack mouth sliding displacement (CMSD) is defined as the difference in vertical displacement of points A and B.

The beam is made of a concrete material. The behavior of the macro-crack, that is initiated from the lower-right part of the notch and propagates in a curved trajectory towards the right side of the lower-right support, is coming from microscale FE computations performed on a $10 \times 10$ mm$^2$ micro-model shown in Figure 6.35b (volume fraction of the aggregates is 60%, data of the aggregate size and ITZ are the same as in the RVE’s existence
6.4 Numerical examples

(a) Macro-model

(b) Micro-model

Figure 6.35 The SEN beam: FE meshes of the macro-model (1219 Q4 elements) and micro-model (5280 T3 elements).

test in Section 6.4.1). The FE discretization is given in Figure 6.35. The load platens are modelled as steel. A plane stress condition is assumed for the micro-model. Material parameters for the constituents of the three-phase microstructure can be found in Table 6.1 except \( c = 0.1 \text{ mm}^2 \). When the maximum macroscale principal stress exceeds 99% of \( \sigma_{\text{ult}}^m \), the crack initiates or propagates in a direction determined using the non-local stress field at the crack tip, Section 6.2.1. To deal with a curved crack as in this example in which the crack direction is not aligned to the micro-sample the algorithm given in Section 6.3.3 is used.

The analysis is performed using the dissipation-based arc-length method [67] together with the sub-stepping scheme proposed in [171]. The sub-stepping technique allows the use of relatively large macroscale load increments which significantly reduces the computational cost of FE computations. The basic idea of this scheme when applied to the multiscale cohesive crack model is whenever the solution for the micro-BVP, Equation (6.11a), could not be obtained (the corresponding macroscale load increment is big), the displacement being imposed on the RVE is divided into sub-steps. It is emphasized that resolving one diverged micro-model with sub-steps is much cheaper than resolving the macro-model with a smaller macro load increment.

The deformed shape of the SEN beam is given in Figure 6.36 in which the
curved crack path that is experimentally observed is captured well. The response of the SEN beam, measured in terms of the load $P$ versus the CMSD, is given in Figure 6.37.

![Figure 6.36](image1)

**Figure 6.36** The SEN beam: deformed configuration of the beam (magnified by a factor of 500) and snapshots of damaging micro-models.

![Figure 6.37](image2)

**Figure 6.37** The SEN beam: load $P$ against CMSD (left) and a typical homogenized cohesive law (right).

### 6.5 Concluding remarks

In this chapter, details concerning implementational and computational aspects of the homogenization-based multiscale crack modelling framework, previously presented in Chapter 5, have been presented. Various issues in-
cluding loading/unloading, macroscopic snapback, arbitrary crack orientation were addressed. Efficient implementation of the master-slave method used to solve nonlinear equations with constraints has been discussed. A probing method was given to compute the macro tangent matrix from the micro stiffness matrix without inversion and partition operations. The given numerical examples show that the method can be used for failure analysis of solids with random heterogeneous microstructures undergoing localized damage. It can also be utilized for designing better materials by adjusting the underlying microstructural constituents’ shape, properties and spatial distribution.
Chapter 7

A continuous-discontinuous multiscale method for cohesive crack modelling*

The crack homogenization method described in the previous chapter is based on the assumption that the energy dissipated prior to microscopic localization is negligible. As a consequence of this assumption, the macroscopic bulk can be modelled as linear elastic without resorting to nested microscopic FE computations. The scheme might be considered as a hybrid homogenization method. The behaviour of the cohesive crack is derived, on the fly, from nested microscopic FE computations, while the behaviour of the macroscopic bulk is, on the contrary, computed \textit{a priori} using conventional homogenization theory.

In this chapter an extension of the multiscale cohesive crack scheme from Chapter 5 is presented in which the behaviour of the macro-crack as well as of the macroscopic bulk are all defined from nested microscopic FE computations. The constitutive law for the macroscopic bulk is derived using the standard continuous/bulk computational homogenization scheme as presented in Chapter 2, Section 2.4. A macroscopic crack is initiated at a macro integration point when the RVE associated with this point shows localization. The cohesive law for the macro-crack is computed based on the cohesive crack homogenization procedure given in Chapter 5. The method introduced in Chapter 5 is further generalized to fit in the new multiscale method. The transition from a bulk homogenization scheme to a crack homogenization scheme is discussed. Details on the algorithm are provided.

An attempt is made here to give a comparison of our method to previous approaches. Comparing to [108] where an embedded localization band was used at the macroscale, we adopt discrete cracks to treat macroscopic localization as done in [15, 115, 116]. Macro cracks are modelled using the extended finite element method (XFEM) (see e.g., [124, 198]) as it is the case in [13, 15] allowing crack path continuity across element boundary. This is an advantage compared to [115, 116] in which crack path continuity across

* Based on [139, 141]
element boundary was not enforced. Different from the aforementioned previous works, our method (and [194]) is applied to random heterogeneous materials (e.g., concrete) for which the RVE cannot be defined as a periodic unit cell as in the case of masonry materials. A unique feature of our method is the move from periodic boundary conditions to other boundary conditions on the RVE at localization. Similar to [15, 108, 115, 116], the initiation/propagation of macro-cracks are derived from the microscale information. The crack direction is, however, computed on the basis of the macroscale stress field. This is in contrast to [15, 108, 115, 116] in which the macro-crack orientation is defined using the microscale information as well.

The layout of this chapter is as follows. In Section 7.1, the multiscale constitutive laws are described. Section 7.2 presents the proposed fully coupled multiscale method. Among various topics, a localization analysis to detect macro-crack initiation, a switch from a full periodic boundary condition to a hybrid periodic boundary condition and a cloning procedure are discussed. Finally some numerical examples are given in Section 7.3 to demonstrate the capabilities of the method.

7.1 Macroscopic model

Considering a macroscopically homogeneous yet microscopically heterogeneous solid as shown in Figure 7.1. The discrete equation for quasi-static equilibrium reads

\[ f_{\text{ext}}^{M} = f_{\text{int}}^{M} = f_{\text{bulk}}^{M} + f_{\text{coh}}^{M} \quad (7.1) \]

with

\[ f_{\text{bulk}}^{M} = \int_{\Omega_{M}} B^{T} \sigma_{M} d\Omega, \quad f_{\text{coh}}^{M} = \int_{\Gamma_{M}} N^{T} t_{M} d\Gamma \quad (7.2) \]

where notations have been introduced in Chapter 6, Section 6.1.

Solving Equation (7.1) requires setting up constitutive relations for Cauchy stress \( \sigma_{M} \) and traction \( t_{M} \). These constitutive relations are herein provided by means of computational homogenization procedures rather than by phenomenological constitutive models. Therefore the burden of the material parameter identification process at the macroscale is alleviated because this process is now shifted down to the microscale where the finding of material parameters for individual constituents is believed to be easier.
7.1 Macroscopic model

Multiscale constitutive models

The behaviour of the macroscopic bulk is given by the following multiscale constitutive equation

\[
\sigma_M = \Psi(\varepsilon_M, \sigma_m)
\]
\[
\delta \sigma_M = D_M : \delta \varepsilon_M
\]

(7.3)

where \(\varepsilon_M\) is the macroscale strain tensor, \(\sigma_m\) is the microscale stress tensor and \(D_M\), a fourth order tensor, is the homogenized bulk tangent. Computation of \(\sigma_M\) and \(D_M\) given \(\varepsilon_M\) (at a bulk integration point) is done via the so called bulk computational homogenization procedure described in Chapter 2, Section 2.4.

The behavior of the macroscale cohesive cracks is described using a multiscale cohesive law that reads

\[
t_M = \Phi([u]_M, \sigma_m)
\]
\[
\delta t_M = T_M \cdot \delta [u]_M
\]

(7.4)

where \([u]_M\) is the displacement jump across the macro-crack and \(T_M\), a second order tensor, is the homogenized cohesive tangent. Providing the displacement jump \([u]_M\) at one cohesive integration point, the corresponding traction \(t_M\) and cohesive tangent \(T_M\) are computed using the cohesive crack homogenization procedure presented in Chapter 5.
The basic idea of the fully coupled multiscale method for cohesive crack modelling is illustrated in Figure 7.2. The entire deformation state of the RVE can be divided into two regimes namely hardening regime and softening regime. The hardening regime (of a micro sample) is transferred to the macroscopic bulk material via the bulk homogenization scheme described in Section 2.4. The softening regime (of a micro sample) is transferred to the macro-crack using the crack homogenization scheme presented in Chapter 5. The method is therefore named a continuous-discontinuous homogenization scheme. The fully FE\(^2\) scheme for cohesive crack modelling is depicted in Figure 7.3 for three-noded triangular elements for sake of simplicity. Representative volume elements that are associated with the bulk Gauss points (GPs) are denoted by bulk RVEs whereas RVEs coupled to cohesive GPs are called cohesive RVEs. From a physical point of view, the proposed multiscale scheme models the transition from micro-cracks into macro-cracks. As long as the micro-cracks do not form a localization band, the microscopic deformation is upscaled to the macroscopic bulk. Only when the micro-cracks bridge and coalesce to form a micro localization band, a macro-crack is initiated at the macroscopic scale. Different stages in the continuous-discontinuous homogenization scheme are discussed in the following subsections.

**Figure 7.2** Coupling between macro- and micro-models in the continuous-discontinuous homogenization scheme. The entire deformation state of a micro sample is represented by the microscale load-displacement \( f_m-u_m \) curve.
7.2 A fully coupled multiscale method for cohesive cracks

Figure 7.3 The fully multiscale homogenization scheme. Initially bulk GPs are coupled with RVEs. When localization occurs in one of the RVEs, a macro-crack is inserted at the corresponding macro-element. Henceforth, cohesive GPs are coupled to RVEs that are cloned from the localized RVE. The bulk GPs of the cracked macro-element follow a secant unloading path. Dotted lines denote periodic boundary conditions.

7.2.1 Hardening regime

The coupling between the bulk Gauss points and RVEs is done via the standard continuous computational homogenization scheme presented in Section 2.4 with periodic boundary conditions for all edges.

7.2.2 Detection of the microscopic limit point

At every converged state of the macroscale problem, a localization analysis, that is based on the homogenized bulk tangent $D_M$, is carried out for all bulk RVEs. This localization analysis is going to be discussed in Section 7.2.6. Once localization is detected in one RVE, say localized RVE, (associated with a bulk GP of a macro-element $e$), the actions given in Box 8 are taken (the discussion is limited to three-noded triangular elements).
Chapter 7  A continuous-discontinuous multiscale method

The initial state of the cohesive RVEs is built using a cloning operation that is described in Section 7.2.4. Note that the macro-crack direction is not coming from microscale information as in [13, 15, 108] but is taken perpendicular to the maximum principal direction as proposed in [194].

**Box 8** Actions to be done when a new crack segment is introduced.

1. A crack segment is inserted to element \( e \) with two new cohesive GPs

2. These two cohesive GPs are henceforth coupled to two RVEs that are cloned * from the localized RVE

3. Sub-triangulating [124, 198] element \( e \) to build new bulk GPs locating on either side of the crack just inserted

4. Compute a secant unloading matrix \( D_{un} \) for the bulk GPs of macro-element \( e \) by temporarily unloading the localized RVE and compute the corresponding homogenized material tangent, Eq. (2.62).

* This is achieved with a cloning operation described in Section 7.2.4.

Step 1 in Box 8 follows the standard algorithm adopted in XFEM. That is, if none of the neighboring elements of element \( e \) is cracked, the crack segment is going through the cracked GP in a direction perpendicular to the maximum principal stress direction. Otherwise, the crack segment is extended from the existing crack tip (e.g., [124, 198]). Note that step 4 in Box 8 becomes more complicated for macro-elements with more than one Gauss point. Without rigorous evidence, we propose to compute \( D_{un} \) for all new bulk GPs from the bulk RVE associated with the cracked Gauss point (e.g., GP of which the associated bulk RVE has been localized). Note also that in two dimensional FE² applications, three-noded triangular elements and bilinear quadrilateral elements with one point quadrature [11] are in favour because they involve the smallest number of RVE computations.

**Remark 7.2.1.** Note that, once inserted, the macro-crack is fixed. This is in contrast to [115] in which the macro-cracks are allowed to change their orientation. This assumption is, however, appropriate for the case considered in this study in which there is no strong damage redistribution at microscale after localization.
7.2 A fully coupled multiscale method for cohesive cracks

7.2.3 Softening regime

For a cracked macro-element, it is assumed that

1. Bulk GPs follow the analytical expression \( \sigma_M = D \epsilon \)

2. Cohesive GPs follow the crack homogenization scheme presented in Chapter 5 with a slightly modified version of the homogenization relation, cf. Equation (6.10)

\[
\mathbf{u}_R = (w-l) \mathbf{C} \cdot \mathbf{t}_M + \mathbf{u}_M + \mathbf{\dot{u}}_{\text{dam}}, \quad \mathbf{C} = \Delta^T \mathbf{D}^{-1} \Delta
\]  

(7.5)

where \( \mathbf{D} \) is a secant tangent matrix that is described later. Note that matrix \( \mathbf{C} \) is computed only once at the crack insertion moment. This is consistent with the assumption that after a localization band has been formed, the surrounding material is unloading elastically. Refer to Figure 7.4 for a graphic illustration of the transition from a microscopic localization band to a macro-crack.

Item 1 indicates that the bulk GPs of a cracked macro-element are no longer coupled to RVEs. This choice has two advantages namely (i) less computational cost and (ii) facilitates the bifurcation of material behavior i.e., the material inside the macro-crack experiences loading at a higher rate when compared to the surrounding bulk material as commonly observed in experiments. However this issue requires further investigation, especially for macro-elements having multiple Gauss points.

The pseudocode of the fully coupled multiscale method for cohesive crack modelling is given in Box 9. Note that this procedure is for three-noded triangular elements only. Although not indicated in Box 9, when the traction \( \mathbf{t}_M \) at a cohesive GP becomes small e.g., 1% of the traction at the moment of crack insertion, the crack becomes traction-free and therefore the cohesive GP is no longer coupled to any cohesive RVE. This reduces the computational cost and allows traction-free cracks even with the exponential damage law given in Equation (2.15).

7.2.4 Cloning operation

A natural choice for the cloning operation is to simply copy the localized bulk RVE to the RVEs that are subsequently used for the cohesive GPs. We
Box 9 Procedure for the fully coupled multiscale crack model.

1. Loop over multiscale macro-elements
   
   a) For a non-cracked element, do
   
   i. Get $\epsilon_M$
   
   ii. Use $\epsilon_M$ as BCs for associated bulk RVE, solve micro-BVP
   
   iii. Compute $\sigma_M$ using Eq. (2.57) and $D_M$ via Eq. (2.62)
   
   b) For a cracked element, using $\sigma_M = D_{un}\epsilon_M$

2. End loop over multiscale macro-elements

3. Loop over cohesive crack segments

   a) Get jump $[u]_M$

   b) Solving Eqs. (2.20)-(7.5) via the iterative scheme (Chapter 5)

   c) Compute traction (Eq. (6.12a)) and cohesive tangent (Eq. (6.12b))

4. End loop over cracks

5. Solving the macro linear system

6. Upon macroscopic equilibrium, do

   a) Loop over critical elements, check eigenvalues of $D_M$

   b) If localization is detected,
      
      i. do actions in Box 8
      
      ii. compute $D$, $l$ and $\dot{u}_{dam}$ in Eq. (7.5)
      
      iii. resolve the macroscopic load step with new crack segment

   c) If no localization,
      
      i. commit state of all RVEs
      
      ii. go to next load increment

---

1 Multiscale macro-elements: elements of macro mesh where the fully coupled CH scheme is applied, see Section 7.2.7

2 With its state being reset to its previous converged values.

3 Critical elements: elements where new crack segments can be initiated.
7.2 A fully coupled multiscale method for cohesive cracks

Figure 7.4 From microscopic localized deformation to an equivalent localization band and finally to a macroscopic crack. Note that the idealization step (1) is not completely correct for a random heterogeneous material. Even after a localization band has been formed, some points in the region outside of the band are still loading.

refer this cloning as standard cloning operation. In this case the $D$ matrix in Equation (7.5) simply equals $D_{\text{un}}$. This works for constant stress elements. However, this choice is facing the following difficulties

1. not general since it does not work for elements with more than one Gauss point (RVE of which GP should be copied?)
2. incompatibility of boundary conditions used for the bulk homogenization scheme and the crack homogenization scheme

We propose herein a new cloning operation by which the aforementioned difficulties are bypassed. The stress field of the localized RVE is known which allows to compute the averaged stresses, $\sigma_{M}^{\text{loc}}$, at the corresponding macro bulk GP. The traction at this GP, denoted by $t_{M}^{\text{loc}}$, is then defined using $t_{M}^{\text{loc}} = \sigma_{M}^{\text{loc}} n$ where $n$ is the normal vector of the macro-crack. The initial state of the RVE used for the newly introduced cohesive GP is defined by loading a micro-sample from undeformed state to $\tau_{M}^{\text{loc}}$ (this is done with small sub-steps to ensure convergence of the Newton-Raphson method utilized to solve the micro BVP) using BCs of the crack homogenization scheme, see Figure 7.5. We call this load control cloning operation. One could argue that parameter $\alpha$ should adopt a value of unity. This choice however encounters divergence problems when $t_{M}^{\text{loc}}$ corresponds to the microscopic peak load. A numerical study of this $\alpha$ parameter is given in the numerical examples.
Figure 7.5 Building the initial state for cohesive RVEs with the load control cloning operation. A force is applied on node 2 whereas other nodes on the right edge are forced to have the same displacement as node 2.

Section (Section 7.3.1). Figure 7.6 illustrates this process for elements having more than one GP.

After the load control cloning operation, the secant matrix $D$ in Equation (7.5) is computed as follows. The deformed cohesive RVE is temporarily unloaded (e.g., by imposing a zero displacement). At the converged state of this unloading step, the material tangent, that is computed using Equation (2.62), is the sought for secant matrix $D$. Note that this unloading state of the cohesive RVE is only needed for computation of the secant matrix and is therefore not saved.

7.2.5 Advantages/disadvantages of the proposed model

The proposed fully multiscale crack model with the new cloning operation offers the following advantages:

1. Applicability to any kind of macroscopic finite elements.
2. Avoid incompatibility issues between BCs of continuous and discontinuous CH scheme.
3. Allows usage of a cohesive RVE which may differ (e.g., size or microstructure) from the bulk RVE.
4. Macroscopic failure criteria to initiate cracks are no longer used.

Item 3 is interesting since it might happen that RVEs for the bulk and RVEs for the cohesive cracks are different in size. This issue requires further investigation. In this thesis, the RVEs for the bulk and for the crack have the
7.2 A fully coupled multiscale method for cohesive cracks

Figure 7.6 Standard cloning operation does not work for macro-elements having more than one GP. The initial cohesive RVE is not copied from any bulk RVE (which RVE should be copied?). Instead the stresses at the cohesive GP, $\sigma^{loc}$, is determined from the bulk stresses at the four GPs, the traction is then computed as $t^{loc}_{M} = \sigma^{loc} n$. The cohesive RVE is made by pulling an undeformed RVE to this traction.

The initiating/propagation of a macro-crack is based on the appearance of strain localization at the microscopic scale. The issue of localization detection in a computational homogenization context has been discussed in [108] where the authors have utilized two criteria that are based on the

same dimension, microstructure and material properties. There are also a few disadvantages related to this fully coupled multiscale model:

1. Extremely high computational expense.
2. Reliance on the macroscopic stress field in determining the crack direction.

The reasons that we are more inclined to the use of a macroscopic crack direction criterion than to a microscopic criterion are (i) determination of the crack direction using macroscopic stresses is fast and efficient, (ii) this criterion is suitable for mode I problems.

7.2.6 Localization analysis

The initiation/propagation of a macro-crack is based on the appearance of strain localization at the microscopic scale. The issue of localization detection in a computational homogenization context has been discussed in [108] where the authors have utilized two criteria that are based on the
acoustic tensor associated with the homogenized bulk tangent and on the homogenized bulk tangent itself. For sake of completeness, both criteria are briefly discussed here.

**Singularity of acoustic tensor criterion** Detection of microscopic localization can be based on the singularity condition of the acoustic tensor that reads

\[
\det(Q) = 0, \quad Q = n \cdot D_M \cdot n
\]  

(7.6)

where \(Q\) is the so-called localization tensor or acoustic tensor and \(n\) is the normal vector to the strain discontinuity surface.

**Limit point criterion** The eigenvalues of the homogenized bulk tangent \(D_M\) are denoted by \(\lambda_{D_M}\). A limit point is reached when the lowest of these eigenvalues vanishes i.e.,

\[
\lambda_{D_M} \leq 0
\]  

(7.7)

For a non-symmetric tangent like \(D_M\) in this manuscript, condition (7.6) may be satisfied before the limit point criterion (7.7) is reached [200]. In this work, we therefore utilize the limit point criterion to initiate/propagate macro-cracks because the cohesive law of macro-cracks is coming from the descending branch of the microscopic stress-strain curve.

**Remark 7.2.2.** In [108, 115], the authors used the limit point criterion for the detection of macro-crack initiation/propagation and an eigenspectrum analysis of the acoustic tensor \(Q\) to define the crack orientation. In this thesis, however, the maximum macroscale principal stress direction is used to define the macro-crack direction. Reasons for this choice have been given in Section 7.2.5. Note that an eigenspectrum analysis of the acoustic tensor \(Q\) is computationally expensive. It deserves future work to extend the current formulation to adopt the eigenspectrum analysis of \(Q\) for determining the macro-crack direction and conduct a comparison of the two approaches.

### 7.2.7 Practical usage of the scheme

Direct application of the continuous-discontinuous CH scheme to every finite element of the macroscopic FE mesh would lead to extreme computational cost. To reduce the cost, we divide the computational domain into
two sub-domains namely the non-critical region and the critical region. To the former, standard continuum elements with effective properties (computed prior to the multiscale simulation) are applied. Multiscale elements (e.g., macro-elements having RVEs coupled to its bulk and cohesive GPs) are used for the latter. Figure 7.7 illustrates the idea. It is emphasized that, in the current implementation, the decomposition of the computational domain into the non-critical and critical sub-domains is performed at the stage of generating the FE discretization for the macro solid and not during the simulation. This assumes knowledge of regions where macro-cracks are likely to develop. This knowledge can be based on experiments or on a preliminary stress analysis. Applying an adaptive homogenization procedure, in the sense that a decomposition of the domain into critical and non-critical domains is performed during the analysis, is an interesting alternative albeit more complicated [56, 93, 183].

7.3 Numerical examples

In this section three examples are provided to investigate the capabilities of the proposed method. In the first example, a simple uniaxial tension test is analyzed to verify the method against a direct numerical simulation (DNS). The goal is to verify whether the continuous-discontinuous CH scheme can capture a continuous “reference” solution. The second example
demonstrates the existence of an RVE for random heterogeneous softening materials when using the proposed multiscale method. Finally, a multiscale crack propagation problem is discussed in the third example. Unstructured finite element meshes used in this section have been generated using Gmsh [54].

In this section a three-phase material, consisting of hard aggregates with a weaker surrounding zone called ITZ (Interfacial Transition Zone) embedded in a soft damaging matrix, is considered, see Figure 4.1, Chapter 4.

### 7.3.1 Verification of the method against DNS

Considering the example described in Figure 7.8 which shows a sample subjected to a uniaxial tensile loading applied on the right edge. The microstructure has a 45% volume fraction of circular aggregates (of which the radius varies from 2.5 mm to 5.0 mm). The width of the ITZ is 0.25 mm. Material parameters of different phases are tabulated in Table 7.1. A plane strain condition is assumed. The macroscopic equilibrium path is traced using standard displacement control with a constant increment of $2 \times 10^{-5}$ mm per load step. The solution (in terms of the load-displacement response measured at the right edge) of the problem given in Figure 7.8 is referred to as the reference solution to which the solution of the same problem but obtained with the proposed fully coupled multiscale model, see Figure 7.9, is compared.

![Figure 7.8](image)

*Figure 7.8* A macro sample in uniaxial tension solved with the bulk homogenization model. Finite element meshes of: macro model (left) and micro model (right). Note that the microstructure shown in the right figure is for the case $d = 10$ mm.

In this example, a considerable amount of energy will be dissipated (responsible for damage initiation in the ITZ) before a localization band is
7.3 Numerical examples

Figure 7.9  A macro sample in uniaxial tension solved with the fully coupled multiscale model: macro-mesh (left) and micro-mesh (right). Rigid plates (Young’s modulus of 10e12 N/mm²) are added to impose BCs since in our PUM code BCs cannot be applied on enriched nodes. The dotted line denotes the crack to be inserted upon satisfaction of a failure criterion.

formed. Therefore, the original multiscale model with elastic behaviour for the macroscopic bulk cannot yield a correct result for this case. The simplicity of this problem enables us to study the main characteristics of the proposed method. The goal of this example is to

- demonstrate the improvement of the new multiscale model (presented in this Chapter) over the original one (presented in Chapters 5 and 6);
- study parameter $\alpha$ in the load control cloning process;
- compare the standard cloning operation and the proposed load control cloning;
- and to demonstrate the performance of the iterative scheme used to solve Equations (2.20)-(7.5).

When a failure criterion is fulfilled (for the original crack homogenization model in Chapter 5, the maximum principal stress criterion was used, and for the fully multiscale model presented in this chapter, the microscopic localization condition has been applied), a vertical crack is inserted in the middle of the center element. Note that the algorithm given in Section 7.2 for three-noded triangular elements can be directly used for four-noded quadrilateral elements used in this example since the deformation is homogeneous. Additionally, due to the homogeneity of the deformation, only one micro-BVP is solved for a bulk GP (stress and bulk tangent is then simply copied to other bulk GPs) and one micro-BVP for a cohesive GP. This
Table 7.1 Material parameters of different phases of the random heterogeneous material.

<table>
<thead>
<tr>
<th></th>
<th>Matrix</th>
<th>Aggregate</th>
<th>ITZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [N/mm$^2$]</td>
<td>25 000</td>
<td>30 000</td>
<td>20 000</td>
</tr>
<tr>
<td>$\nu$ [-]</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$\kappa_1$ [-]</td>
<td>5e-06</td>
<td>0.5</td>
<td>2.8e-06</td>
</tr>
<tr>
<td>$\gamma$ [-]</td>
<td>0.999</td>
<td>0.999</td>
<td>0.999</td>
</tr>
<tr>
<td>$\beta$ [-]</td>
<td>1500</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>$c$ mm$^2$</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Remark 7.3.1. The fully coupled multiscale solution was verified against the reference solution (obtained with the continuous/bulk CH scheme). In fact, for this simple problem, it can be seen that the reference solution is identical to the DNS solution (in the DNS, a periodic boundary condition is directly applied on the $d \times d$ microstructural sample), see Figure 7.12.

The performance of the full FE$^2$ scheme with the standard cloning operation is analyzed and the results are depicted in Figure 7.13. Although the

ad hoc implementation dramatically reduces the computation time and thus speeds up the implementation validation process of multiscale methods.

Firstly, the $10 \times 10$ mm$^2$ sample ($d = 10$ mm) is considered. The load-displacement diagrams obtained with the original multiscale formulation and the new scheme (also referred to as full FE$^2$) are given in Figure 7.10 together with the reference solution. The figure demonstrates the inability of the original scheme to accurately model the damage process prior to crack initiation. This makes the original FE$^2$ solution more brittle than the reference solution. Actually the post peak behaviour of the original FE$^2$ solution is shifted to the left with respect to the reference solution. It is emphasized that the post-peak portion of the load-displacement curve obtained with the original scheme is virtually parallel to the one of the reference solution. This indicates that the crack homogenization described in Chapter 5 correctly extracts the softening behaviour out of the microscopic sample. The proposed fully coupled FE$^2$ scheme gives a result that is in good agreement with the reference solution. The distribution of the nonlocal equivalent strain that drives the microscopic damage is depicted in Figure 7.11.
deformation in the macro-sample is homogeneous, simply copying the localized bulk RVE to the cohesive RVE gives a result that is more brittle than the reference solution. This might be explained by the fact that the macro-sample is much weaker with the presence of a discrete crack governed by a softening traction-separation law. Support for this explanation is given in the following paragraph.

In the load control cloning operation, the initial state for the cohesive RVE is obtained by loading an undeformed RVE to a traction \( t = \alpha t_{\text{loc}}^M \). A numerical study on the value of this parameter \( \alpha \) is carried out and the result
Chapter 7 A continuous-discontinuous multiscale method

Figure 7.12 Sample made of a multiphase material–load-displacement curves: reference solution, the DNS solution and the new fully multiscale solution (load control cloning with $\alpha = 0.97$).

is given in Figure 7.14. For $\alpha = 0.999^*$, a brittle response like the solution obtained with the standard cloning operation is obtained. The same observation is made for $\alpha = 0.99$ although the response is less brittle. Solutions that are in good agreement with the reference solution are obtained with $\alpha = 0.98$ and $\alpha = 0.97$. The introduction of a discrete crack with a softening cohesive law ($\alpha = 0.999, \alpha = 0.99$) makes the sample much weaker compared to the damaging sample without a crack. With $\alpha = 0.98, \alpha = 0.97$, the homogenized cohesive laws have a hardening part thus enabling the cracked sample to still carry more load after crack initiation. These two types of homogenized cohesive laws, one with only a descending branch and one with an ascending branch (albeit small) and then a descending one are given in Figure 7.13b. For $\alpha$ being smaller than 0.97, responses that are more ductile than the reference solution have been acquired. To consolidate the above observation, let us consider another case with $d = 15$ mm as shown in Figure 7.15 (with material parameters given in Table 7.1 except $c = 0.05$ mm$^2$). The analysis on different values for $\alpha$ is shown in Figure 7.16. For $\alpha = 0.97$ and $\alpha = 0.98$, softening cohesive laws are obtained thus making the continuous-discontinuous solution more brittle than the reference continuous solution. A homogenized cohesive law with a hardening part is obtained for $\alpha = 0.95$, hence a solution that properly captures the

$^*$A value of unity of $\alpha$ led to divergence of the Newton-Raphson procedure.
7.3 Numerical examples

Figure 7.13 Brittle response obtained with the standard cloning operation (a) and homogenized cohesive laws (b) obtained with the standard cloning and load control cloning ($\alpha = 0.97$).

The reference solution has been obtained.

From the above analysis the parameter $\alpha$ seems to be undesirably problem dependent. To explain the reason and give a hint on the value this parameter should have, we plot the reference solutions of two samples $10 \times 10$ mm$^2$ and $15 \times 15$ mm$^2$ together in Figure 7.17. The load-displacement curve of the $15 \times 15$ mm$^2$ sample (with $c = 0.05$ mm$^2$) has a sharp peak while the one that corresponds to the $10 \times 10$ mm$^2$ sample (with $c = 0.1$ mm$^2$) has a blunt peak. This is because larger values of $c$ lead to damage zone that is spread throughout the micro-sample and therefore more energy is dissipated before a localization band forms. Figure 7.18 explains why, for the same $\alpha = 0.97$, the multiscale continuous-discontinuous solution for the $10 \times 10$ mm$^2$ sample is close to the reference solution while it is not the case for the $15 \times 15$ mm$^2$ sample. Due to a sharp peak, only a small displacement ($\Delta u$) imposed on the cohesive RVE will result in a jump to a point on the softening branch (see the right figure of Figure 7.18), hence the homogenized cohesive law does not have a hardening part. On the contrary, with a blunt peak, a small displacement imposed on the cohesive RVE will result in a jump to a point that is still on the hardening branch (see the left figure of Figure 7.18), hence the homogenized cohesive law has a hardening part. Note that when a small macro load step is used, for the $15 \times 15$ mm$^2$ sample and $\alpha = 0.97$, a good solution is obtained as well, see Figure 7.19.

It is emphasized that with the load control cloning for $\alpha \neq 1$ the traction continuity condition, referred to as the time continuity in [148], is not fulfilled. However in this simple problem no deterioration in the convergence
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Figure 7.14  Numerical study of $\alpha$ used in the load control cloning operation ($d = 10$ mm). Note that for $\alpha = 1$, the load control cloning step failed due to divergence.

Figure 7.15  The $15 \times 15$ mm$^2$ sample with $c = 0.05$ mm$^2$. The right figure shows the non-local equivalent strain contour.

Figure 7.16  Numerical study of $\alpha$ for a $15 \times 15$ mm$^2$ sample: load-displacement diagrams (left) and a close-up view (right).
rate of the Newton-Raphson scheme utilized to solve the macroscopic BVP has been observed.

The performance of the iterative scheme introduced in Chapter 5 used to solve the microscopic BVP Equation (2.20) and the homogenization equation (7.5) is given in Figure 7.20. Although this kind of analysis has been given in Chapter 6 for voided microstructures, we present such an analysis here because (i) the homogenization equation has been changed and (ii) it is used for a random microstructure. For each macroscopic Newton-Raphson iteration and for each cohesive Gauss point, one has to solve the micro-BVP (for cohesive GPs) \( p \) times. Figure 7.20 shows that most of the time \( p = 2 \) which indicates good convergence characteristic of the iterative scheme. Further-
Figure 7.19 With small macro load step size, $\alpha = 0.97$ also gives a good solution for the $15 \times 15 \text{mm}^2$ sample.

Figure 7.20 Performance of the iterative scheme used to solve the microscopic BVP and the homogenization equation.

more, one has to solve $m$ times the micro-BVP for $m$ bulk RVEs which are not yet localized. Note that in this simple problem, where there is only one element along the crack path, $m = 0$ after a macro-crack has been initiated.

The problem is now also analyzed with three-noded triangular elements as shown in Figure 7.21. The bottom figure verifies the implementation of the multiscale scheme for both bilinear quadrilateral elements and constant
7.3 Numerical examples

Finally, the unloading of the bulk material surrounding the crack (for the $15 \times 15 \text{ mm}^2$ sample but now with a refined mesh) is demonstrated in Figure 7.22. It can be observed from this figure that after a macro-crack is initiated the surrounding bulk material unloads.

7.3.2 RVE’s existence test

In order to demonstrate the existence of an RVE for softening materials when using the proposed continuous-discontinuous homogenization
Figure 7.22 Snapshots of the uniaxial tension bar for the $15 \times 15$ mm$^2$ sample: (a) at the peak load and (b) at the end of simulation.

Figure 7.23 RVE’s existence test: macro mesh (left) and micro samples (right). The centered element (shaded element) is the multiscale element while the other two elements are assumed to be rigid. Length unit is mm.

scheme, let us consider the example shown in Figure 7.23. A uniaxial tension bar discretized into three four-noded quadrilateral elements is considered. Three micro models of size $10 \times 10$ mm$^2$, $15 \times 15$ mm$^2$ and $20 \times 20$ mm$^2$ are investigated. The volume fraction of aggregates, its range of radius and thickness of the ITZ are taken identical to the ones given in the first example (see Section 7.3.1). Material parameters of the microstructural constituents can be found in Table 7.1 except $c = 0.2$ mm$^2$ to make a comparison with results reported in Chapter 6. The macro-sample is loaded using displacement
control and a plane strain condition is assumed. The sub-stepping scheme in [171] has been used to ensure convergence of the microscopic BVP when the macroscopic kinematics (the strain tensor $\epsilon_m$ in case of bulk homogenization and the displacement jump $\|u\|_M$ in case of crack homogenization) downscaled to the microscale are large (e.g., the micro-BVP could not be solved in one single increment). The existence of an RVE is verified by the convergence of the load-displacement response (measured at the right edge of the macro-sample) with increasing the size of the micro-samples. Note that this RVE’s existence test has been given in Chapter 5 for voided materials and in Chapter 6 for random heterogeneous materials in the context of the crack homogenization scheme.

Figure 7.24 Objectivity of the macroscopic response with respect to different adopted micro-samples.

Figure 7.24 plots the load-displacement curves (the load control cloning is adopted with $\alpha = 0.999$) and the corresponding homogenized traction-separation curves. As can be seen, increasing the size of the micro-samples makes the macroscopic responses converging. Note that the $10 \times 10$ mm$^2$ sample is too small to be statistically representative for the microstructure, that is why its solution deviates somewhat from the solutions of the larger samples. By comparing this result with the one given in Figure 6.22, that has been obtained with the original FE$^2$ scheme, we observe that the post-peak responses of the $15 \times 15$ mm$^2$ and $20 \times 20$ mm$^2$ samples are not as close as they are in Figure 6.22. We attribute this small discrepancy of the post-peak responses obtained with the continuous-discontinuous CH scheme to the difference between the hardening regimes (e.g., the nonlinear part of the
pre-peak regimes) which were not taken into account in the discontinuous CH scheme (pre-peak response was assumed to be linear elastic). It should be noted that for random microstructures, a statistical analysis (herein, for a certain size, only one realization has been made) should be performed. The averaged responses would then be closer to each other.

### 7.3.3 Crack propagation
Multiscale crack propagation is studied by the problem given in Figure 7.25. In order to minimize the computational cost, a small micro sample with a microstructure having a low aggregate density (30%) is chosen. This micro sample is therefore not an RVE according to its definition and the term RVE used in this example is only to be consistent with the terminologies previously introduced in this chapter. The analysis is performed under a plane stress state with displacement control. Only one crack is allowed in this example. When the external load is sufficiently large, a crack is initiated at the notch and propagates in a direction perpendicular to the applied forces. To reduce the computational expense, only one row of elements ahead of the notch are defined as critical elements i.e., elements upon which the proposed continuous-discontinuous homogenization scheme applies (see Section 7.2.7). For the other elements, standard continuum elements with effective elastic properties are utilized. Material parameters of the microstructural constituents are given in Table 7.1. The initial state of the cohesive RVEs are built using the load control cloning operation with $\alpha = 0.97$. Finite element meshes of the macro model and the micro model are given in Figure 7.26. The micro-mesh consists of 8600 three-noded triangular elements (T3 elements). The macro-mesh shown in Figure 7.26, denoted henceforth mesh1, consists of 1560 T3 elements in which there are 32 macroscopic critical elements leading to 32 bulk micro problems. After a crack segment is initiated, there are two new cohesive micro problems introduced into the system and the bulk RVE of the cracked element is disabled. When the crack reaches the top edge, there are 64 cohesive micro problems and no bulk micro problem. For a mesh sensitivity analysis, two other macroscopic meshes, depicted in Figure 7.27, are studied as well. The same RVE regarding size and microstructure has been used for mesh2 and mesh3. The load-displacement (measured at point A, Figure 7.25) curves are given in Figure 7.28. The first macro-mesh, mesh1, is simply too coarse to model crack propagation accurately. It should be mentioned that the load drops are due to the fact that the crack grows element-wise in our XFEM implementa-
7.3 Numerical examples

This observation has also been reported in [157] regarding monoscale crack growth simulations. With refined macro-meshes, mesh2 and mesh3, a converged response has been obtained. Small load drops are still present which can be removed if a XFEM formulation with a crack tip element (i.e., the crack can end inside an element) such as the one presented in [157] is adopted. The deformed shape of the wedge (mesh1) is given in Figure 7.29 together with snapshots of some damaging cohesive RVEs.

![Figure 7.25 Multiscale wedge splitting test: geometry, boundary conditions of the macro sample (left) and the underlying microstructure (right). Unit of length is mm. The dotted line denotes the crack to be initiated and propagated. The width of the notch is 5 mm. Note that the chosen micro sample is too small to be representative.](image1)

It is noteworthy to say that we did not present a DNS for this problem because such a DNS simply exceeds the currently available computer power.
Chapter 7 A continuous-discontinuous multiscale method

Figure 7.27 Finite element meshes of the macro model: mesh2 contains 2258 T3 elements (52 critical elements) and mesh3 consists of 2863 T3 elements (72 critical elements).

Figure 7.28 Multiscale wedge splitting test: load-displacement (measured at point A) response.

7.4 Concluding remarks

A fully coupled multiscale method for modelling failure of random heterogeneous quasi-brittle materials has been presented. The method is considered as a continuous-discontinuous CH scheme for multiscale modelling of failure of quasi-brittle materials. The classical bulk/continuous CH theory
has been used for the bulk to model the pre-cracked material. Upon micro-
scopic localization, a macroscopic cohesive crack is introduced of which be-
aviour is determined using the so-called crack/discontinuous CH scheme.
Microscopic failure that is represented by a localization band of finite width
is upscaled to a macroscopic crack to model macroscopic failure. Details on
the formulation as well as on its computer implementation have been dis-
cussed. The new model offers the following advantages compared to the
cohesive crack homogenization method described in chapters 5 and 6 (i)
macro crack initiation is now based on microscale information, and (ii) the
pre-failure hardening part is included. The method is therefore suitable for
materials that show diffusive damage in addition to a dominant localization
band. A simple verification problem was given in which the proposed mul-
tiscale method has been successfully validated against a reference solution
for mode I failure. It was shown numerically that the homogenized cohesive
law should have a (small) ascending (hardening) part in order for the
continuous-discontinuous multiscale solution to capture the continuous re-
ference solution. Convergence of the macroscopic responses upon increasing
the size of micro-samples has been demonstrated. Finally a crack growth
simulation was presented and mesh-insensitive results were obtained.
Chapter 8

Applications

In this chapter computational techniques discussed in previous chapters are combined together to devise a macro-meso-micro three-scale model for concrete materials. Due to limited computer resources available, only the concept of the three-scale model is given and we resort to two two-scale models. The first model is a macro-micro two-scale model which is applicable to mortar materials. The micro model represents the microstructure of the mortar (hardening cement paste) which is obtained with the cement hydration model described in Chapter 3. The second model is a meso-micro two-scale model in which the coarse scale model is now a mesoscale model (aggregate/matrix two-phase material) and the fine scale models consist of a microscale model (hardening cement paste) for homogenizing the behaviour of the cohesive cracks in the mesoscale matrix phase and another microscale model (representing the microstructure of the mesoscale interface transition zone) for homogenizing the interface between the mesoscale aggregate and matrix. In order to deal with heavy computations, we present a parallel implementation of the multiscale model described in Chapter 5 based on the concept of a processor farming model.

The remainder of the chapter is structured as follows. Section 8.1 presents the parallelization of the multiscale cohesive crack model. Section 8.2 presents the two-scale models. Section 8.3 describes the three-scale model for concrete followed by some numerical examples given in Section 8.4.

8.1 A parallel implementation of the multiscale model

Computational homogenization methods, due to nested FE computations, are very time consuming. One efficient way to speed up the CH simulation time is the utilization of parallel computers. Parallelization of the standard CH methods (to model bulk materials) has been developed in literature, see for instance [85, 173]. In this section, we present a parallel implementation

* Based on reference [140]
of the crack CH model which has been presented previously in Chapters 5 and 6.

The processor farming model [112] is chosen to parallelize the multiscale crack model presented in Chapters 5 and 6. The basic idea of the processor farming model is that tasks are distributed by one farmer processor to several worker processors, and results are sent back to the farmer. For efficiency, the extra time spent on communications must be small compared to the time spent processing each task and each of the CPUs must be ready approximately at the same time. This model fits well for CH simulations where the solution of the macro model requires the solution of a larger number of independent micro models. This explains why this model has been chosen to parallelize computational homogenization (CH) codes, refer to for instance [13, 85, 106, 173].

![Diagram of the farmer model](image)

**Figure 8.1** The farming model for the case $n_{RVE} > n_{CPU}$. The RVEs are divided into blocks of which one block contains $n_{CPU}$ RVEs. RVEs in every block are solved in parallel.

### 8.1.1 General procedure

The resulting parallel multiscale model is given in Figure 8.1. Let us assume that there are $n_{CPU} + 1$ processors and there are $n_{RVE}$ RVEs. The coarse scale model is solved using the farmer processor named CPU0. The fine scale models are handled using $n_{CPU}$ processors left. We present an implemen-
tation for the case in which $n_{\text{RVE}} > n_{\text{CPU}}$. This is suitable for running the simulation on personal computers with a few processors and on moderate clusters. Since $n_{\text{RVE}} > n_{\text{CPU}}$, one worker processor has to solve more than one RVE. Therefore, we have decided to store the state (which consists of nodal values and history variables for all integration points of the RVE mesh) of all RVEs at the farmer processor CPU0. Before solving an RVE, the correct state is sent to the corresponding worker processor. This results in a somewhat higher overhead due to extra communications between the farmer and the worker processors (in addition to the standard communications that send the macro displacement jump vectors to the worker CPUs and receive the homogenized tractions and tangents from worker CPUs). The parallel implementation is given in Box 10. As can be seen, the assembly of the stiffness matrix and internal force vector (of the cracks) for the macroscopic FE model is divided into three steps. In the first step, a loop over all cohesive Gauss points (GPs) is done to collect all the displacement jumps and states. In the second step the collected data are sent to the worker processors. After doing their job (solve the RVE problems), the worker processors send the tractions and tangents back to the farmer processor. In the final step, actual computation of the stiffness matrix and internal forces is done using this information. We refer to [133] for more details.

The master and worker processors communicate through a so-called message passing context using the Message Passing Interface (MPI) [49] library. A parallel implementation of the continuous CH model described in Chapter 2, Section 2.4 using the processor farming model has also been done. Details are given in [133]. Note that a parallel implementation of the continuous-discontinuous CH model given in Chapter 7 is not carried out.

Remark 8.1.1. Assume that there are four worker CPUs and 6 RVEs. Then, the first four RVEs labelled RVE$_1$, RVE$_2$, RVE$_3$ and RVE$_4$ are assigned to the four processors. When these four RVEs have been solved, the two left RVEs, RVE$_5$ and RVE$_6$, are assigned to CPU1 and CPU2 and solved simultaneously. Let us assume further that the solution time of RVE$_1$ is longer than the solution time of other RVEs. In this case, while CPU1 is still solving RVE$_1$, CPU2, CPU3 and CPU4 are free. Only when RVE$_1$ is solved, one continues with RVE$_5$ and RVE$_6$. This is a drawback of our current implementation to be improved in a future work.
**Box 10** Processor farming model for parallelizing the multiscale crack model.

1. **Initialization:** coarse scale mesh, BCs, $n_{CPU}$ etc.

2. **Assembly for crack**
   
   a) **Data collection:** for one crack segment, loop over cohesive GPs
      
      i. Collect jumps into one array, $jump$
      
      ii. Collect states into one array, $state$
   
   b) **Exchange data**
      
      i. Send data ($jump$, $state$) to worker processors
      
      ii. Solve RVEs on worker processors in parallel
      
      iii. When an RVE solved, compute $t_M, T_M$, update its state
      
      iv. Collect RVE data ($t_M, T_M, \sigma$) into $tract, tangent, state$
      
      v. Send $tract, tangent, state$ back to CPU0
   
   c) **Assembly process:** for one crack segment, loop over cohesive GPs
      
      i. Retrieve corresponding traction, tangent from $tract, tangent$
      
      ii. Compute $f_{coh}^M, K_{coh}^M$
      
      iii. Assemble them to the global quantities
      
      iv. Update the state of all RVEs using $state$

3. **Assembly for bulk elements:** done sequentially (CPU0)

4. **Solve the macroscopic system of equations** (CPU0)

5. **Convergence:** commit state for all RVEs and write to files (CPU0)

$\alpha$ represents the state of an RVE.

Steps 2-4: one Newton-Raphson iteration for a given macro load step.

Step 2b: performed block by block, one block contains $n_{CPU}$ RVEs.

### 8.1.2 Theoretical speed-up factor

Let us recall that there are $n_{CPU}$ worker CPUs. The number of RVEs can be generally defined as $n_{RVE} = \alpha n_{CPU} + \beta(n_{RVE} - \alpha n_{CPU})$ where $\alpha, \beta$ are positive integer numbers defined by
8.1 A parallel implementation of the multiscale model

\[ \alpha = n_{RVE} \backslash n_{CPU}, \quad \beta = \begin{cases} 1 & \text{if } n_{RVE} > \alpha n_{CPU} \\ 0 & \text{otherwise} \end{cases} \tag{8.1} \]

where the symbol \( \backslash \) denotes the integer division operator. For example, if there are 8 CPUs and 100 RVEs, then \( \alpha = 12 \) and \( \beta = 1 \). Assuming that the time to solve all RVEs is the same and denoted by \( t_{RVE} \).

The computation time of a sequential computation is given by

\[ t_{seq} = n_{RVE} t_{RVE} \tag{8.2} \]

where the time spent on the macroscopic problem has been neglected.

Since there are \( \alpha \) blocks of \( n_{CPU} \) RVEs of which RVEs in one block is solved in parallel, the computation time of the parallel computation is given by

\[ t_{par} = \alpha t_{RVE} + \beta t_{RVE} \tag{8.3} \]

where the time spent on data communication has been assumed to be small.

The speed-up factor \( s \) is therefore defined as

\[ s \equiv \frac{t_{seq}}{t_{par}} = \frac{n_{RVE}}{\alpha + \beta} \tag{8.4} \]

For \( \beta = 0 \), \( s = n_{CPU} \). For \( \beta = 1 \),

\[ s = \frac{n_{RVE}}{\alpha + 1} \approx n_{CPU} \quad \text{when } n_{RVE} > n_{CPU} \times n_{CPU} \tag{8.5} \]

which indicates that the speed-up factor is about the number of worker processors when the number of RVEs is significantly larger than the number of worker processors i.e., \( n_{RVE} > n_{CPU} \times n_{CPU} \). For the example with 8 CPUs and 100 RVEs, \( s = 100/13 \approx 8 \). However, with 8 CPUs and 25 RVEs, the speed-up factor is only \( s = 25/4 \approx 6 \). The speed-up factor \( s \) as defined in Equation (8.4) is the maximum theoretical speed-up factor that can be achieved. In case that there are RVEs which take more time to be solved than the rest, the obtained speed-up factor is smaller than the number of worker processors.
8.2 Two-scale models for concrete

Assuming that the finest scale of interest is the scale in which the microstructure of hardening cement paste is visible (the so-called microscale). The reader is referred to [40] where, among other things, nanoscale modelling of concrete has been presented. There are three two-scale models that can be developed for concrete namely a macro-meso model (this model has been used in Section 6.4.4), a macro-micro model and a meso-micro model. In this section, the two latter are discussed.

8.2.1 A macro-micro two-scale model

In Figure 8.2 a macro-micro two-scale model for mortar materials is given. Description of the macro and micro model is presented in what follows.

![Figure 8.2 A macro-micro two-scale model for mortar materials.](image)

**Macroscale model** At the macroscopic scale, a homogeneous material is adopted. Failure at this scale is represented by discrete cracks of which behaviour is determined from nested microscopic FE computations in the framework of the discontinuous CH model given in Chapters 5 and 6.

**Microscale model** The microstructure of the micro model is the hardening cement paste which is generated using the cement hydration model described in Chapter 3. Microscale failure is modelled with the regularized isotropic damage model presented in Chapter 2, Section 2.2.1.
8.2 Two-scale models for concrete

8.2.2 A meso-micro two-scale model

Figure 8.3 depicts a meso-micro two-scale model that can be used to study the mechanical behaviour of concrete samples at mesoscale in which the microstructures of the cement paste and of the ITZ are taken into account.

**Mesoscale model** Instead of using a three-phase (matrix-aggregate-ITZ) mesoscale model as described in Chapters 4, 5 and 6, in this chapter, a two-phase (matrix-aggregate) mesoscale model in which the ITZ is modelled with zero-thickness interface elements, see Figure 8.3. Matrix cracking is treated using the multiscale cohesive crack model given in Chapter 5 whilst matrix/aggregate debonding is modelled with the multiscale adhesive crack model described in Chapter 5.

**Microscale models** There are two microscale models, the first one is for homogenizing the cohesive crack running through the mesoscale matrix phase and the second one is used for homogenization of the ITZ (a sort of heterogeneous material layer). Basically, the microstructure of these two micro-models can be generated using the cement hydration model described in Chapter 3. For details concerning the ITZ, refer to [16, 178] and references herein. Microscale failure mechanism is modelled with the regularized isotropic damage model presented in Section 2.2.1.
8.3 A three-scale model for concrete

The materials have been presented in previous chapters enables the development of a macro-meso-micro three-scale model for concrete as described in what follows, refer also to Figure 8.4. Macroscopically the concrete sample is homogeneous with a propagating crack (macro-crack) of which behavior (e.g., the extrinsic cohesive law) is derived from a mesoscale model. At the mesoscale, concrete is modelled as a two-phase material that consists of hard aggregates embedded in a soft matrix. Meso-scale failure is accompanied by meso-cracks in the matrix. The behavior of the meso-cracks is coming from a so-called microscale model. The microscale model is the hardening cement paste presented in Chapter 3. The macro/meso scale coupling, which represents a transition from meso discrete cracks to macro discrete cracks, is treated using the method given in [194] (see also Section 2.5.2) whereas the meso/micro scale coupling is handled with the multiscale method presented in Chapters 5 and 6. Although this three-scale model is conceptually possible, it is extremely demanding regarding the computational cost it incurs. Therefore, it has not yet been implemented.

![Figure 8.4 A macro-meso-micro three-scale model for concrete.](image)

8.4 Numerical examples

In this section two numerical examples are given. In the first example, the performance of the implemented parallel multiscale code is presented. Sec-
ondly, an example that demonstrates the use of the macro-micro two-scale model described in Section 8.2.1 is presented.

### 8.4.1 Parallel performance

**Continuous CH model** In order to assess the parallel performance of the continuous CH model, let us consider the uniaxial tension test given in Figure 8.5. There are 25 four-noded quadrilateral elements with 100 GPs hence 100 RVEs. The RVE, which represents the microstructure of concrete at mesoscale, corresponds to a 45% volume fraction of aggregates (of which radius varies from 2.5 mm to 5.0 mm). The width of the ITZ is 0.25 mm i.e., 10% of the smallest diameter of the aggregates. Note that this value is not realistic (the ITZ’s thickness in reality is much smaller). This value was chosen in order to have a FE mesh that can be solved within a reasonable amount of time. Each RVE is discretized by 6112 three-noded triangular (T3) elements. A plane strain condition is assumed for the RVEs. The material parameters of different constituents making up the RVE are given in Table 7.1. The maximum number of worker CPUs is eight. The example is first solved with the sequential code and then with the parallel code in which the number of worker CPUs is varied from 2 to 8. The simulation has been performed on a desktop with eight cores and a shared memory architecture.

![Figure 8.5](image)

**Figure 8.5** Parallel performance test for the bulk CH model: macro FE mesh (left) and micro FE mesh (right).

Figure 8.6 gives the performance comparison between a sequential computation and a parallel computation. With four worker processors, a speed-up factor of 3.68 was obtained (the maximum speed-up factor is 4). However using eight worker processors, a lower speed-up factor was observed. This is due to the reduced memory bandwidth for a shared memory machine.
when there are more worker processes. This drop in performance would disappear when a distributed memory machine is used.

![Figure 8.6](image_url)

**Figure 8.6** Numerical performance of the parallel continuous CH model. Elapsed time for one macroscale load increment and the numerical speed-up factor defined as the ratio between the sequential time and the parallel time.

Since the number of RVEs is fixed in the continuous CH model, the above analysis applied to one load increment can be extrapolated to the whole simulation i.e., a speed-up factor of 3.6 is observed (four worker CPUs are used) for the whole simulation.

**Discontinuous CH model** To test the parallel performance of the crack CH model, the problem given in Figure 8.7 is considered. When the macroscale maximum principal stresses exceed the tensile strength of the material, a vertical crack is inserted in the middle of the macro mesh. There are four cohesive GPs (two GPs for one crack segment), thus there are four RVEs of which microstructural constituents are described in the previous example for the continuous CH model. A plane strain condition is assumed for the RVEs.

Figure 8.8 plots the runtime for one load increment (all four RVEs are active) versus the employed number of worker processors. With two worker processors, a speed-up factor of 1.95 was obtained and with four worker processors, a factor of 3.6 was observed i.e., speed-up factors which are closed to the theoretical value have been obtained.

Since in a multiscale crack simulation the number of RVEs is increasing as the crack propagates the speed-up factor for the entire simulation cannot be equal to the speed-up factor for one load step. In order to test the parallel performance of the discontinuous CH model for a crack propagation problem, the wedge splitting test, presented in Chapter 6, Section 6.4.3, is considered.
8.4 Numerical examples

Figure 8.7 Parallel performance test for the crack CH model: macro FE mesh (left) and micro FE mesh (right).

Figure 8.8 Numerical performance of the parallel crack CH model. Elapsed time for one macroscale load increment and the numerical speed-up factor defined as the ratio between the sequential time and the parallel time.

In the beginning there is no RVE (no crack is initiated yet). At a certain load step when the macroscopic maximum principal stress exceeds the tensile strength, a crack is initiated in the specimen. When it propagates through the specimen it cuts 31 elements. The number of RVEs thus increases from 0 to 62. The DNS runtime was 14 hours whereas the sequential multiscale simulation took 3.25 hours (4.3 times faster than the DNS). Using eight worker CPUs, the parallel multiscale analysis took 0.86 hours i.e., 16.3 times faster than the DNS and 3.8 times faster than the sequential multiscale simulation.

In Figure 8.9, the parallel performance is given by comparing the total runtime of the sequential and the parallel simulation. As can be seen, the speed-up factor is about four i.e., only half of the number of worker CPUs. This can be explained by looking at Figure 8.10 which shows that the speed-
up factor per load step varies from step to step. The solution time for one coarse scale load step is defined by the number of Newton-Raphson iterations, the number of fine scale BVPs that has been solved and the solution time for one fine scale BVP. It should be emphasized that the number of fine scale BVPs needed to be solved is larger than the number of RVEs. This is because, for one RVE, we had to solve the fine scale BVP Equation (6.11) a couple of times until the homogenization relation Equation (6.11) is fulfilled. Note that this is simply a first result on the parallel performance of the discontinuous CH model for crack propagation simulations obtained with eight worker CPUs. Using a significantly larger number of worker CPUs e.g., 62 CPUs the parallel performance behaviour would be different. However, it is clear that a significant speed-up will be certainly obtained.
8.4.2 Two-scale analysis of mortar samples

In order to illustrate the macro-micro two-scale model presented in Section 8.2.1, the problem as described in Figure 8.11 is considered. The microstructure is the Z slice of a 3D cement paste that was hydrated for 28 days, see Section 3.3 in Chapter 3. The FE discretizations are given in Figure 8.12. Note that a relatively coarse mesh (13,912 T3 elements) is used to discretize the microstructure to reduce the computational cost. Material parameters of the microstructural phases are given in Table 3.2 except $\beta = 500$ and $c = 2 \times 10^{-6}$ mm$^2$. Displacement control is used to trace the macroscopic equilibrium path and a plane strain assumption is adopted for the microscopic model. When the maximum principal stress at the macroscopic sample exceeds 0.0503 N i.e., 99% of the ultimate load of the micro sample, a vertical crack is inserted at the middle of the sample.

Figure 8.11 A mortar sample in uniaxial tension test: macroscale (left) and microscale (right).

Figure 8.12 A mortar sample in uniaxial tension test: FE meshes consisting of three bilinear elements of the macroscale sample (left) and microscale model (right). The thick line denotes the crack.
Remark 8.4.1. In the current implementation of the crack CH model, periodic boundary conditions are treated using a periodic FE mesh i.e., every node on the bottom edge will have a marching partner on the top edge. Using the algorithm given in Box 2, Section 3.2.3, to eliminate pore elements and any isolated elements would result in a non-periodic mesh. Therefore, in this example, we have used a mesh in which the pore is discretized (Young’s modulus of the pore is 0.01 N/mm$^2$) so that periodicity is ensured. It should be emphasized that in [96], a novel treatment of periodic BCs has been presented by which a periodic RVE mesh is no longer required.

![Figure 8.13](image)

Figure 8.13  Mortar sample in uniaxial tension test: load displacement diagram (left) and damage distribution in the microstructure (right).

Figure 8.13 plots the macroscopic load displacement response and the localization band in the microstructure.

8.5 Concluding remarks

In this chapter, a parallel implementation of the multiscale cohesive crack model has been given. A simple analysis for determining the maximum theoretical parallel speed-up was carried out. Numerical examples have shown that the speed-up of the parallel continuous CH model is very close to the theoretical value. For the crack CH model, it was demonstrated that with only eight processors, an significant gain in computation time compared to direct numerical simulations has been obtained.

Two two-scale models for concrete materials have been presented. The concept of a macro-meso-micro three-scale model for concrete was also introduced.
Chapter 9

Conclusions

Failure of many natural and engineering materials occurs at different length scales. Proper multiscale methods that are able to bridge failure mechanisms occurring at various length scales have proved useful not only to predict more accurately the macroscopic behavior of materials but also to provide alternatives to conventional material design approaches. In this dissertation, such a method has been developed firstly for a cohesive crack and then for an adhesive crack. The so-called multiscale cohesive laws for these cracks are completely derived from the mechanical behavior taking place at microscopic scale. The salient points of the research reported in this thesis are summarized in what follows.

The first contribution of this work (Chapter 3) is a fully numerical framework to study the mechanical behavior of hardening cement pastes. This micro-mechanical model is analyzed in a multiscale framework presented in Chapter 8.

Homogenization-based methods rely on the crucial assumption of the existence of an RVE (Representative Volume Element). In this thesis (Chapter 4) it has been shown that, by homogenizing towards a cohesive law, instead of a stress-strain relation, an RVE does exist for softening materials. This is achieved with the failure zone averaging scheme which is based on the observation that a microscopic localization band has a constant width (related to the internal length scale of the material under investigation) regardless of the RVE size.

The cornerstone of this work (Chapter 5) is the development of a homogenization-based multiscale framework to model cohesive failure of heterogeneous solids. By the introduction of a cohesive crack at macroscale, with behaviour coming from nested microscopic finite element computations, the macroscopic boundary value problem is well-posed and the numerical solution is insensitive with respect to the discretization of the macroscopic solid. By the virtue of the failure zone averaging technique, the homogenized response is objective with respect to the RVE size. Therefore, an objective homogenization method has been presented for strain localization
problems. Contrary to other coarse-graining methods for failure modelling where the direction of the microscopic failure band determines the direction of the macroscopic crack, the presented computational homogenization (CH) formulation determines the macroscopic direction based on the macroscopic stresses. Also presented in this chapter is a multiscale model for modelling heterogeneous material layers. The theory given in Chapter 5 is further developed in Chapter 6 where an algorithm has been presented to handle macroscopic cracks with an arbitrary direction.

The multiscale method presented in Chapter 5 was built upon the assumption that the energy dissipated prior to microscopic localization is negligible. In Chapter 7, a continuous-discontinuous computational homogenization procedure has been given in which the aforementioned assumption is relaxed. The basic idea of the method is that constitutive behaviour of the bulk material as well as that of the cohesive crack is all determined from nested microscopic finite element computations. Macro-cracks are initiated based on the appearance of microscopic localization instead of using a macroscopic failure criterion as in Chapter 5. Although computationally expensive, the continuous-discontinuous homogenization scheme is more accurate than the scheme described in Chapter 5 for problems in which the energy dissipated prior to microscopic localization is significant.

Chapter 8 combines the materials described in the previous chapters to devise multiscale models for concrete materials namely (i) a macro-meso-micro three-scale model for concrete and (ii) a macro-micro two-scale model for mortar materials. To accelerate multiscale simulation, parallelization of the developed multiscale models is presented.

**Future perspective**

It is obvious that the developing field of multiscale failure modelling of heterogeneous materials cannot be covered in one single thesis. Many aspects have therefore not been studied here. Relevant unresolved issues are discussed in the following.

The development given in this thesis has been confined to quasi-static loading conditions which limits its applicability. Extension of the present theory to impact loadings in order to study the dynamic fracture of heterogeneous materials is a direction of future research.

Although the existence of a representative volume element has been confirmed for concrete material in tensile loading and to some extent shear loading, the actual size of such a RVE has not been reported in this thesis. How-
ever this can be done without major difficulties by combining the ideas in
this dissertation with a statistical analysis.

The computational multiscale model developed in this thesis is currently
restricted to small-scale simulations due to the extreme computational cost
it incurs. Since the major part of the computation is spent in solving the
microscopic boundary value problems, any numerical technique that could
quickly solve the microscopic boundary value problems would dramatically
reduce the computation time of the proposed multiscale model. Reduced
order models (ROMs) applied for the microscopic model provide a promis-
ing avenue. Parallel computing in combination with ROM-based techniques
would make large-scale multiscale simulations applicable.

Although the proposed methods have been verified against direct numer-
ical simulations, they have not been validated against experiments. One rea-
son is the lack of a proper value for the gradient damage parameter $c$ utilized
at the fine scale model.

Yet another unresolved issue is the one of handling snapback at the mi-
croscale. Although no snapback at the microscale has been observed for the
utilized damage model and chosen parameters, a robust computational ho-
mogenization method should be able to handle both macroscopic and mi-
croscopic snapback.

Yet another interesting topic of future research that has been identified
during the course of this work is multiscale inverse analysis for determin-
ing material parameters of the microstructural constituents by matching the
macroscale behavior (obtained with a multiscale model) to an experimental
results at different levels. Modified objective functions need to be derived
for this.

The multiscale framework presented in this thesis might be extended to
study multiphysics problems such as moisture transportation in cracked
concrete samples in which the microstructure of concrete is taken into ac-
count.

A logical direction for future work is to make the continuous-
discontinuous CH scheme (see Chapter 7) adaptive. This will make the
scheme applicable to problems where the crack path is not known $a$ priori.
References


References


References


References


Propositions

1. The failure zone averaging technique presented in this dissertation allows for the definition of representative volume elements for softening materials.

2. Although computationally expensive, direct numerical simulations are indispensable for verification of multiscale methods.

3. It usually takes a long time for novel numerical models developed in research institutes to become commercially available.

4. Assumptions often limit the applicability of the methods that are built on them. Properly chosen ones, however, save a huge amount of computational expense.

5. The homogenization process only makes sense when one can find a length scale at which material constants of all heterogeneities can be determined experimentally in a direct or indirect manner.

6. The adequacy of a homogenization-based multiscale method relies not only on the coarse/fine scale linking but also on the accuracy of the modelling technique used for the fine scale model.

7. Collaboration between people around the world is one of the nicest things in the academic environment.

8. Foreign PhD students working in the Netherlands usually do not speak Dutch not only because Dutch is a difficult language to learn but also because Dutch people speak English so well.

9. Asian people usually find it hard to integrate themselves into a Western society.

These propositions are regarded as opposable and defendable, and have been approved as such by the supervisor, Prof. dr. ir. L.J. Sluys.
**Stellingen**

1. De in dit proefschrift behandelde homogenisatietechniek - genaamd "failure zone averaging technique" - staat de definitie van een representatief volume element toe.

2. Ondanks de extreme rekenijden, zijn directe numerieke simulaties onontbeerlijk voor de verificatie van multischaal methoden.

3. Het duurt meestal lang voordat nieuwe numerieke modellen, ontwikkeld in onderzoeksinstellingen, commercieel beschikbaar worden.

4. Aannames beperken in het algemeen de toepasbaarheid van de modellen die daarop gebaseerd zijn. Echter, wanneer zorgvuldig gekozen kunnen ze je zeer veel rekenijden besparen.

5. Homogeniseren heeft alleen zin als men een lengteschaal kan vinden waarop relevante eigenschappen van alle aanwezige heterogeniteiten direct, dan wel indirect, experimenteel kunnen worden bepaald.

6. De betrouwbaarheid van een op homogenisatie gebaseerde multischaal methode wordt niet alleen bepaald door de relaties tussen de twee schalen, maar ook door de nauwkeurigheid van modelleren van de fijnste schaal.

7. Het samenwerken met mensen over de hele wereld is één van de leukste aspecten van een academische omgeving.

8. Het feit dat buitenlandse studenten, werkzaam in Nederland, vaak geen Nederlands spreken ligt niet alleen aan de lastig te leren taal, maar komt ook doordat Nederlanders zo goed Engels spreken.

9. Aziaaten vinden het vaak moeilijk om te integreren in de westerse samenleving.

Deze stellingen worden opponeerbaar een verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotor, Prof. dr. ir. L.J. Sluys.
Curriculum vitae

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A great part of the content of this thesis has been published in peer reviewed international journals and conferences as listed below.

Journal papers


**Conferences**


