Computational Modeling of Failure in Composite Laminates
Computational Modeling of Failure in Composite Laminates

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Summary

Computational Modeling of Failure in Composite Laminates

There is no state of the art computational model that is good enough for predictive simulation of the complete failure process in laminates. Already on the single ply level controversy exists. Much work has been done in recent years in the development of continuum models, but these fail to predict the correct failure mechanism in cases where matrix cracking in off-axis plies is part of the global mechanism (Section 2.1). The way forward is to model matrix cracks as true discontinuities in the displacement field, in which case the orientation of the cracks can easily be controlled. A mesh-independent representation with partition of unity based methods or, similarly, the phantom node method is to be preferred, because with these methods cracks can initiate and grow at arbitrary locations in the model, wherever the stress field gives rise to it (2.2).

This requires an initially rigid mixed mode cohesive law. Unfortunately, straightforward formulation of such a law leads to a singularity; the traction is not uniquely defined for zero crack opening and zero damage. Robustness of the simulation requires that this singularity is removed from the description. Two methods exist that do this. Firstly, it is possible to relate the cohesive traction not only to the displacement jump, but also to the stress in the surrounding material. Secondly, one can start from a cohesive law with a finite initial stiffness and then apply a shift to the origin to mimic initially rigid behavior. With both methods a cohesive law is derived that satisfies the Benzeggagh-Kenane relation for mixed mode fracture energy (2.3 and 2.4).

The constitutive model for the single ply is completed with a damage/plasticity law for shear nonlinearity and a continuum damage model for fiber failure (2.5 and 2.6). The ply model can be used as a building block for analysis of complex failure mechanisms in laminates.

For full-laminate analysis, an additional failure process is possible, namely delamination. The proposed laminate model consists of a single layer of elements for each unidirectional ply, interconnected with interface elements. These interface elements are equipped with a cohesive law for delamination (3.1). Notably, the interaction between the phantom node method in the plies and the interface elements is accurate without updating the interface elements, particularly when a nodal integration
scheme is used (3.2). A complicating aspect of laminate analysis, is that matrix cracking may occur in a distributed fashion because of mutual constraint between the plies. It is possible to model many cracks with the phantom node method. However, the number of cracks must be limited with a minimum crack spacing parameter to keep the problem well posed and to allow for coalescence of cracks (3.3).

Because laminate failure is a highly nonlinear process, a carefully designed solution algorithm is indispensable to bring simulations to a successful end. Sharp snapbacks may occur because the stiff fibers may unload suddenly when failure progresses through the laminate. In order to follow the equilibrium path through these snapbacks, an arclength method is needed. The dissipation-based arclength method is used for this purpose, because it is robust and generic. The formulation is extended for cases with both permanent deformations and damage (4.1). Adaptive time stepping is crucial (4.3) and in some cases a modified Newton-Raphson scheme is to be preferred (4.4).

The discontinuities that are represented matrix cracks, which may be numerous, are inserted during the computation. This is handled after equilibrium has been found. After crack propagation, equilibrium is sought again before the next time step is entered, but multiple crack segments may be introduced at once (4.2).

The framework is validated against experimental observations for several laminate cases (5). Subcritical damage consisting of delamination and matrix cracks is generally captured well. Different failure mechanisms can be described and the appropriate one is ‘chosen’ automatically because the different processes are incorporated realistically. The fiber failure model lacks a representation statistical strength distribution of the fibers and is therefore not predictive in brittle cases where the strength in fiber direction is a key parameter.

This work has resulted in a robust integrated framework for computational modeling of failure in composite laminates. The numerical results are objective with respect to discretization. Different failure processes and their interaction are represented such that the simulations not only provide insight in when the laminate fails, but also in how it fails.

F.P. van der Meer
Samenvatting

Numerieke Modellering van het Bezwijken van Composietlaminaten

Er is tot op heden geen computermodel dat goed genoeg is om voorspellende simulaties te doen van het complete bezwijkproces in composietlaminaten (gelaagde materialen met sterke vezels; in elke laag hebben de vezels een andere oriëntatie). Al op het niveau van een enkele laag bestaat controverse. De laatste jaren is veel gewerkt aan het ontwikkelen van continuum-modellen (waarin schade wordt uitgesmeerd over een band), maar deze kunnen het juiste bezwijkmechanisme niet voorspellen wanneer matrix-scheuren doorslaggevend zijn in lagen waarin de vezels schuin zijn ten opzichte van de belastingsrichting (Sectie 2.1). De oplossing hiervoor is om matrix-scheuren te modelleren als echte discontinuïteiten in het verplaatsingsveld. Dan kan de oriëntatie van de scheuren worden gecontroleerd. De voorkeur gaat uit naar recente technieken waarmee de scheur door de elementen kan lopen, zoals de methode met zogenaamde phantom nodes. Hiermee is het niet nodig om vooraf te zeggen waar de scheuren zullen optreden, wat natuurlijk voordelig is voor wie voorspellende berekeningen wil doen (2.2).

Deze benadering vraagt om een bijzondere materiaalwet die de scheuropening regelt, namelijk een cohesieve wet die initieel oneindig stijf is in mixed mode. Helaas is de meest voor de hand liggende formulering hiervoor niet numeriek stabiel door een singulariteit die optreedt in de initieel onbeschadigde scheur. Maar er bestaan twee methoden om de singulariteit te verwijderen. Ten eerste is het mogelijk om de spanning in de omgeving van de scheur in de formulering te betrekken. Ten tweede kan een eindige stijfheid aangenomen worden, waarna met een transformatie een oneindige stijfheid ge-imiteerd kan worden. Voor beide technieken is in dit proefschrift een cohesieve wet afgeleid die resulteert in gedrag dat overeenkomt met experimenteel waargenomen gedrag voor de beschouwde materialen (2.3 and 2.4).

Het constitutieve model voor de individuele laag in een laminaat is vervolgens gecompleteerd met beschrijvingen voor niet-lineaire vervorming onder afschuiving en voor vezelbreuk (2.5 and 2.6). Het aldus opgebouwde model is een bouwsteen voor analyse van complexe bezwijkmechanismen in laminaten.

Voor de analyse van complete laminaten met meerdere lagen, is nog een ander bezwijkproces van belang, namelijk delaminatie (scheurvorming tussen de lagen). Het voorgestelde model voor het complete laminaat bestaat uit een enkele laag
elementen per laag in het materiaal, en zogenaamde *interface elementen* die de verbinding tussen de verschillende lagen representeren. Deze interface elementen zijn uitgerust met een cohesieve wet zodat ze kunnen ‘beschadigen’ (3.1). Een opvallende observatie is dat het voor numerieke nauwkeurigheid niet noodzakelijk is om eventuele informatie over *phantom nodes* door te geven aan de interface elementen, wat het gemak van implementatie ten goede komt (3.2). Een complicerende factor voor de analyses is dat heel veel parallele matrix-scheuren kunnen voorkomen. Dit zorgt voor numerieke problemen die pragmatisch opgelost worden door een minimale afstand tussen twee scheuren in dezelfde laag voor te schrijven (3.3).

Omdat het bezwijken van laminaten een sterk niet-lineair proces is, is het ontwerpen van een robuust numeriek schema van groot belang. De kans dat een berekening voortdurend crasht is aanzienlijk, ook als er geen programmeerfouten zijn gemaakt. Om het grillige evenwichtspad te kunnen volgen, is de recent ontwikkelde *dissipation-based arc length* methode zeer geschikt. In dit proefschrift is deze methode uitgebreid voor gevallen waarin zowel permanente vervormingen als scheuren optreden (4.1). Verder is het essentieel dat de tijdstapgrootte tijdens de berekening kan worden aangepast (4.3) en is het in sommige gevallen nuttig om een niet-exacte linearisering te gebruiken (4.4).

De discontinuïteiten die matrix-scheuren representeren, ontstaan en groeien tijdens de berekening. Omdat met scheurgroei eigenlijk het numerieke probleem opnieuw wordt geformuleerd moet dit op een speciale plaats in het algoritme worden gedaan. Vanwege de grote hoeveelheid scheuren in laminaten is dit in dit proefschrift op een nieuwe manier aangepakt (4.2).

Het complete model is getest ten opzichte van waarnemingen die elders bij experimenten gedaan zijn (5). De ontwikkeling van de schade in het laminaat als de belasting wordt opgevoerd is met bevredigende nauwkeurigheid gelijk in simulaties en experimenten. Het model kiest uit verschillende bezwijkmechanismen voor de meest waarschijnlijke, doordat de verschillende relevante processen elk realistisch worden gesimuleerd. In het model voor vezelbreuk, echter, wordt geen rekening gehouden met de statistische verdeling van de sterkte van de vezels, terwijl dit in sommige gevallen wel van belang is.

Dit onderzoek heeft geresulteerd in een robuust en nauwkeurig computermodel waarmee het bezwijken van composietlaminaten gesignaleerd kan worden. Verschillende bezwijkprocessen en hun interactie zijn gemodelleerd zodat het model niet alleen inzicht geeft in wanneer het laminaat bezwijkt, maar ook in hoe dat gebeurt.

F.P. van der Meer
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Frans van der Meer,
August 2010
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Chapter 1 Introduction

1.1 Background

The rise in availability and power of computers over the last decades has been enormous, which has led to a great advance of numerical methods in science and engineering. Nowadays, with the available tools, many things of interest can be computed without too much complication. In the field of mechanics, an example of this is linear stress analysis. All one needs is the geometry and boundary conditions of the problem at hand plus a few material properties that can be established beyond reasonable doubt. It may take some pain to set everything up, but in principle the tools are available that will help one find a solution consisting of displacements and stresses, of great practical use. But many other things of interest remain out of reach. In mechanics, the area of consensus is abandoned when moving towards the analysis of the failure process. The simulation of initiation and propagation of damage in materials is a topic of ongoing research. Here, it is less clear what are the essential parameters and how they can be obtained and there are different concepts for how to represent cracks numerically, each with their own advantages and disadvantages. Moreover, there is often a danger that the computation crashes due to ill-convergence of the numerical algorithms before the virtual material has broken.

A particular challenge exists in the modeling of failure in high performance materials. These materials derive their properties from their specific microstructure: processes on the microlevel govern to a large extent the global failure behavior. There is a separation between the scale on which these processes occur and the scale of interest of the engineer. This poses a challenge for the developer of computational models. Much detail must be included to model the relevant processes accurately, but, on the other hand, too much detail will inflate computational costs excessively. Therefore, there is need for smart numerical techniques that include the relevant processes efficiently. We want a model that can be relied upon as to give reasonable results, but which does not have to be waited upon for weeks before those results are computed.

A composite laminate is such an high performance material. A laminate is a layered material, and composite in this case means that each layer in turn is composed of two materials: fibers (e.g. glass or carbon) and matrix (e.g. epoxy). From this description, the multiscale nature of the material is directly apparent, different levels of observation can be distinguished, see Figure 1.1. The load bearing work in
Chapter 1 Introduction

Microlevel Mesolevel Macrolevel

Matrix Fiber Plies Laminate

Figure 1.1 Three levels of observation for composite laminates

laminates is done by the fibers which have a high stiffness and strength, while the matrix material functions in keeping the fibers together. As such the laminate as a whole exploits the strength and stiffness of the fibers, while the poor resistance of individual fibers or fiber bundles with respect to bending is eliminated. In this thesis, only laminates with unidirectional layers (or *plies*) are considered, i.e. the fibers are long and straight and inside the ply all fibers are oriented in the same direction.

Composite laminates are widely applied as a structural material in aircraft and wind turbines. Moreover, thanks to their high strength and stiffness with relatively low weight, composites are promising for application in slender civil engineering structures such as high rise buildings and bridges. The potential of composites however, is not fully exploited yet, partially because prediction of the reliability of composite structures is difficult. This leads to high safety factors and/or extensive testing. The number of tests on components and structural parts that is required to achieve safety certification of a typical large composite airframe, for example, is of the order 10,000 [19]. If more reliable computational analysis were possible, this could reduce the number of tests and hence the certification costs considerably. Moreover, fast computational tools could aid the material researcher in improving the material and give the engineer more freedom to optimize the design.

The main complicating aspect for laminate failure analysis is that different processes may occur during failure. Plasticity and cracking of the matrix material may occur, as well as fracture of fibers in tension or kinking of fibers in compression, possibly accompanied by debonding in the fiber-matrix interface. Matrix failure can be classified as *delamination* when it occurs between the plies or as matrix cracking or ply splitting when the crack is oriented through the thickness of the ply. Here, the term *transverse matrix cracking* is generally used for cracks oriented perpendicular to the load direction and *splitting* for cracks in load direction. Reliable failure analysis of a composite structure must include a representation of each of the possible processes as well as their interaction. Prediction of onset of the failure processes is not sufficient, because initial local failure does not necessarily lead to loss of integrity of the structure. Especially after matrix failure, the load bearing capacity of
1.1 Background

Splitting
Matrix cracking
Delamination
Fiber failure

Figure 1.2 Schematic representation of the different failure processes in tensile failure of a laminate with a circular hole.

the composite is not necessarily exhausted, since stress may be redistributed over the fibers. Therefore, failure analysis has to be progressive, i.e. the progression of failure through the material should be simulated.

Not only does the presence of different failure processes complicate the development of computational models, it also deepens the need for them. The strength of a laminate with particular geometry and layup depends on the interplay between the different processes, and simple mechanical tools are not able to predict how the competing mechanisms interact. This becomes for instance manifest in the fact that strength does not linearly scale with specimen size. Upon doubling the thickness of a laminate, it does not necessarily become two times as strong. In fact, the type of failure may change completely when the thickness of the plies is changed [29]. These size effects in laminates cannot be explained with established models that bring into account the statistical strength distribution (statistical size effect) or the relative size of the fracture process zone with respect to the geometry (deterministic size effect). Therefore, either each particular geometry and load case has to be tested individually, or numerical models must me employed that predict all relevant processes accurately. As of yet, such numerical models do not exist.

The objective of this study is to improve the state of the art of the computational modeling of progressive failure of composite laminates. The focus is primarily on the mesolevel, but the challenge thereby is to represent the relevant micromechanical processes correctly. We will work towards a framework in which different failure processes are taken into account. The numerical reliability of the different components will be tested, as well as the ability to reproduce the real material behavior in non-trivial cases. In order to complete these tests, computational robustness is a big issue. To formulate accurate models is one thing, but to embed them in algo-
rithms that will avoid abortion of the simulation due to ill-convergence is at least as challenging, and this is therefore one of the main issues in the development of the framework.

1.2 Thesis outline

In the remainder of this chapter the necessary background for the thesis will be presented, introducing some of the key concepts and reviewing recent literature.

In Chapter 2, a constitutive model for the elementary ply will be presented. This model includes matrix cracking, fiber failure, and shear nonlinearity. It is shown how the continuum approach fails to represent matrix cracking correctly in simple tests, which constitutes the main motivation for the central innovation in this thesis work: the mesh independent-representation of straight matrix cracks with the phantom node method. Much attention is given to the formulation of cohesive laws for robust analysis.

Next, in Chapter 3, the model for the elementary ply will be extended for application in full laminate analysis. The constitutive model for delamination is presented and the interaction between the phantom node cracks in the ply and the interface elements is discussed. Moreover, in laminate analysis, matrix cracking may occur as distributed cracking, which is also addressed.

In Chapter 4 the focus is moved from the constitutive modeling to the algorithmic aspects of the designed numerical framework. This is actually a parallel topic to the development of the constitutive model as presented in Chapters 2 and 3. But because of the fundamentally serial structure of a book, we place it after those two chapters.

Finally, in Chapter 5, the model is tested on real life cases. The numerical reliability of the different components is verified in Chapters 2 and 3, but the comparison with the real observations of laminate behavior is left to this last chapter. Failure experiments on notched specimens with different geometry and layup are simulated to assess whether this framework allows for reliable prediction of laminate failure.

1.3 The finite element method

The work in this thesis is executed in the framework of the finite element method [46, 8]. To be specific, the finite element method is applied for solving the quasi-static equilibrium equation. Here static means non-dynamic, considering that dynamic effects are neglected, i.e. the inertia term is removed from the momentum balance equation. The quasi prefix is used because we are dealing with failure, which is obviously not static in the common sense that nothing changes. Boundary conditions (applied loads or prescribed displacements) are incremented step by step, and these
1.3 The finite element method

Increments are commonly referred to as time steps, although there is no real time in the analyses.

The fundamental unknown is the displacement field. In each time step the displacement field that satisfies equilibrium as well as the essential boundary conditions is approximated by solving the discretized weak form of the equilibrium equation, which is written as a set of equations

\[ f_{\text{int}} = f_{\text{ext}} \]  

(1.1)

where the external force vector \( f_{\text{ext}} \) contains nonzero values only for nodes on which an external force is applied, and the internal force vector \( f_{\text{int}} \) is a function of the displacement field.

In Equation (1.1), the order of the problem has been reduced by discretizing the displacement field with a finite set of degrees of freedom and an equally sized set of interpolation functions or shape functions. The shape functions are defined such that the degrees of freedom can be interpreted as nodal displacements. The nodes are defined in a mesh which divides the problem domain into elements. With the shape function matrix \( N \) and nodal displacement vector \( a \), the displacement field \( \mathbf{u} = \{u_x, u_y, u_z\} \) is expressed element-wise as:

\[ \mathbf{u}(\mathbf{x}) = N(\mathbf{x})a \]  

(1.2)

with

\[ N = \begin{bmatrix} N_1 & 0 & 0 & \ldots & N_n & 0 & 0 \\ 0 & N_1 & 0 & \ldots & 0 & N_n & 0 \\ 0 & 0 & N_1 & \ldots & 0 & 0 & N_n \end{bmatrix} \]  

(1.3)

\[ a^T = \{a_{1x}, a_{1y}, a_{1z}, \ldots, a_{nx}, a_{ny}, a_{nz}\} \]  

(1.4)

where \( n \) is the number of nodes of the element.

The strain field is defined with the strain nodal displacement matrix \( B \) as

\[ \varepsilon = B(\mathbf{x})a \]  

(1.5)

with \( B(\mathbf{x}) = LN(\mathbf{x}) \) and

\[ L^T = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ 0 & \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial x} \\ 0 & 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{bmatrix} \]  

(1.6)

Stress \( \sigma \) is a function of strain \( \varepsilon \),

\[ \sigma = \sigma(\varepsilon) \]  

(1.7)
which can be nonlinear and history dependent. This relation, the constitutive law, describes the material behavior. The simplest constitutive law is Hooke’s law:

\[ \sigma = D^e \varepsilon \]  

(1.8)

where \( D^e \) contains the constant elastic stiffness moduli of the material.

With Equations (1.5) and (1.7), the stress field can be computed from the (history of) the nodal displacements. The left hand side of the equilibrium equation (1.1) is evaluated from the stress field in a loop over the elements:

\[ f^{\text{int}} = \sum_e M_e \int_{\Omega_e} B^T \sigma \, d\Omega \]  

(1.9)

where \( \Omega_e \) is the element domain and \( M_e \) maps the element vector to the corresponding entries in the global vector. To keep the notation compact, in the remainder of this thesis the assembly of element integrals \( \left[ \sum_e M_e \int_{\Omega_e} \ldots \right] \) is written as an integral over the global domain \( \left[ \int_{\Omega} \ldots \right] \). The fact that the \( B \) matrix from Equation (1.5) reappears in Equation (1.9) is related to the Galerkin approximation method [46].

Because \( f^{\text{int}}(a) \) is typically nonlinear, the set of equations in (1.1) cannot be solved for \( a \) directly. The solution is found iteratively with the Newton-Raphson procedure. In each iteration a linearized system is solved. The solution vector is updated in iteration \( j \) with

\[ a_j = a_{j-1} + K_{j-1}^{-1} (f^{\text{ext}} - f^{\text{int}}(a_{j-1})) \]  

(1.10)

where \( K_{j-1} \) is the global tangent matrix evaluated at \( a_{j-1} \):

\[ K_{j-1} = \frac{\partial f^{\text{int}}}{\partial a} \bigg|_{a=a_{j-1}} \]  

(1.11)

Obviously, in computational practice, evaluation of Equation (1.10) does not involve inversion of the global tangent matrix and subsequent contraction with the residual vector. Rather, a direct or iterative solver is used to evaluate \( K^{-1}(f^{\text{ext}} - f^{\text{int}}) \). The update is repeated until the desired level of accuracy is obtained. Then we proceed to the next time step.

The global tangent matrix \( K \) is evaluated in a loop over the elements. For the relations above, it takes the form of

\[ K = \int_{\Omega} B^T D B \, d\Omega \]  

(1.12)

where \( D \), the material tangent, is a linearization of the constitutive law:

\[ D = \frac{\partial \sigma}{\partial \varepsilon} \]  

(1.13)
1.4 Computational modeling of failure of materials

The integrals in Equations (1.9) and (1.12) which are both defined over the element domain are evaluated numerically in a loop over integration points.

Under the conditions that the relation $f^{int}(\mathbf{a})$ is smooth and the starting point is sufficiently close to the solution it can be proved that the Newton-Raphson procedure converges quadratically. Unfortunately, in highly nonlinear simulations the condition of having to start ‘sufficiently close’ may be too tight for practical time step sizes. Moreover, smoothness is generally not ensured. For instance, nonlinear material laws that have different loading/unloading behavior result in a not continuously differentiable relation between force and displacement. In these cases, one may lose quadratic convergence. And even worse, it is not guaranteed that a solution will be found at all. This is a major concern for users and programmers of nonlinear finite element methods. The issue of robustness, which will be addressed repeatedly in this thesis is related to the convergence of the Newton-Raphson procedure.

1.4 Computational modeling of failure of materials

In this section, some of the key concepts in computational modeling of failure of materials are reviewed. Different methods for the modeling of cracks can be subdivided into two categories: the continuum approach and the discontinuous approach. In the continuum approach, the crack is smeared over a band with finite width. This is conceptually appealing, because the intact material is already modeled as a continuum, and then it is convenient if the failure of the material can be represented in the same model. The discontinuous approach however, in which the crack is modeled as a jump in the continuum, does justice to the elementary notion that a crack is not just a weaker kind of material but rather a new interior boundary.

1.4.1 Continuum models

The continuum models fit directly into the finite element framework presented in Section 1.3. They are implemented in the relation between stress and strain, Equation (1.7).

**Plasticity** The nonlinear material law with perhaps most history in finite element modeling is based on the theory of plasticity [42]. This theory has its root in metals analysis, and is built on the idea that deformation can be decomposed in an elastic part and a permanent (or plastic) part. The basic form of the constitutive law with plasticity is

$$
\sigma = D^0 (\varepsilon - \varepsilon^p)
$$

(1.14)
Chapter 1 Introduction

Typically, the plastic strain $\varepsilon_p$ is unknown and computed such that the stress satisfies a certain criterion. This makes Equation (1.14) an implicit set of equations which in most cases has to be solved iteratively with the so-called return mapping algorithms [112].

For modeling of failure, the stress criterion can be formulated such that the stress must vanish upon increasing plastic strain.

**Damage** A more straightforward option is offered by the continuum damage theory [61]. Here, the basic idea is that the stiffness of the material decreases as a consequence of the reduction of the effective cross section when microcracks appear. The simplest formulation, assuming isotropic stiffness degradation is written as

$$\sigma = (1 - \omega)D^\varepsilon \varepsilon$$

where $\omega$ is the damage variable, which grows from 0 to 1 during failure. Generally, the stiffness degradation is computed explicitly from the strain, which grants continuum damage the advantage over plasticity of implementational simplicity and algorithmic robustness.

Practically, the main difference between plasticity and damage is in the unloading of the material. In the case of plasticity, constant $\varepsilon_p$ gives unloading with the initial stiffness, while in the case of damage, constant $d$ gives secant unloading (see Figure 1.3).

**Regularization** Continuum models for failure suffer from severe mesh-dependency. In softening, the nonlinear behavior tends to localize in a single row of elements. The amount of energy that is dissipated in the crack that is smeared over this band depends on the size of the element, vanishing in the limit of very fine discretization.

This can be mitigated with the crack band method, in which the local stress strain behavior depends on the element size as first proposed by Bažant and Oh [4]. However, this does not solve the mesh sensitivity problem completely; element shape
1.4 Computational modeling of failure of materials

and orientation still influence the solution. More advanced localization limiters such as non-local [5] and gradient models [12, 96, 97], which introduce an internal length scale are to be preferred for reliable accurate representation of softening material behavior. These methods however, require a very fine mesh in the failure zone and considerable implementation effort. Another option is to introduce a rate dependent term [130], which has physical meaning for high rate problems, but can also be used artificially with quasi-static problems to resolve the mesh dependency problem.

1.4.2 Discontinuous models

The alternative to smearing a crack over the continuum is to insert a discontinuity in the displacement field. Although this is a more intuitive approach to failure, since displacements really are discontinuous over a crack, it requires more fundamental changes to the finite element formulation. One way or the other, the kinematical formulation has to be adapted to accommodate the discontinuity.

To control the amount of energy that is dissipated in the crack as it propagates and to remove the singularity from the stress field at the crack tip, cohesive forces are applied on the crack surface, following early work by Barenblatt [3]. This means that a second constitutive law is introduced besides the constitutive law for the continuum. This cohesive law relates the cohesive traction \( t \) to the size of the displacement jump \( ||u|| \):

\[
t = t (||u||) \tag{1.16}
\]

The cohesive law can, just like the continuum models, be based on plasticity and/or damage. It does not require special regularization because it is acting on a surface instead of in a volume.

**Interface elements** The most straightforward solution is to have the discontinuity between the elements. Duplicate nodes are used along the crack path to describe a jump in the displacement field (see Figure 1.4. The cohesive forces can be defined on a node to node (lumped) basis [91, 138], or in a continuous interface element [28, 110]. These two are connected through the fact that the often used nodal integration scheme in the continuous interface element renders it essentially similar to the lumped elements.

The interface element consists of two surfaces which are connected to adjacent solid elements. Initially the two surfaces coincide, but they may be driven apart mechanically. The displacement jump is defined as the difference between the displacement field of the two surfaces, which are in turn defined with standard finite
element interpolation functions from Equation (1.2):

\[
[u] = \bar{N} \left\{ \begin{array}{c} a_{\text{top}} \\ a_{\text{bottom}} \end{array} \right\}
\]  

(1.17)

with

\[
\bar{N} = [ \begin{array}{cc} N & -N \end{array} ]
\]

(1.18)

The contribution of the interface element to the internal force vector is then defined as an integral over the interface surface \( \Gamma_i \):

\[
f^{\text{int}} = \int_{\Gamma_i} \bar{N}^T t \, d\Gamma
\]

(1.19)

and the contribution to the global tangent matrix likewise as

\[
K = \int_{\Gamma_i} \bar{N}^T T \bar{N} \, d\Gamma
\]

(1.20)

where

\[
T = \frac{\partial t}{\partial [u]}
\]

(1.21)

**Partition of unity method** An increasingly popular class of methods for modeling of cracks is based on enrichment of the solution basis with discontinuous functions, referred to as PUFEM [82], XFEM [86] or GFEM [117]. Melenk and Babuška [82] introduced the partition of unity finite element method as an easy way to include information about the problem being solved to the finite element basis. Exploiting the partition of unity property of the finite element shape functions, any function can be added to the basis in order to improve its approximability. This includes the possibility to add a discontinuous function for the modeling of cracks, which
1.4 Computational modeling of failure of materials

Figure 1.5 A discontinuity running through the elements with the partition of unity or phantom node method. The enriched nodes are indicated with a circle.

has been done first by Belytschko and Black [7] and Moës et al. [87]. In this way, a discontinuity is running through the elements (see Figure 1.5), which obviously offers more flexibility for the crack path than interface elements. In the original publications, asymptotic functions are used for enrichment around the crack tip to approximate the singular stress field. Alternatively, it is possible to add cohesive tractions on the crack surface, as proposed by Wells and Sluys [132] and Moës and Belytschko [86]. In this case the singularity is removed from the stress field.

In this method, the displacement field is defined as the sum of two independent fields, one of which is multiplied with the Heaviside step function $H$:

$$u(x) = Na + H\tilde{N}a$$

(1.22)

where $\tilde{a}$ are additional degrees of freedom defined only on the nodes of the elements that contain the crack and $H$ is equal to 1 on one side of the crack and equal to 0 on the other side (see Ref. [132]). The displacement jump is defined on the cracked surface $\Gamma_c$ as

$$[u](x) = N\tilde{a}, \quad x \in \Gamma_c$$

(1.23)

Phantom node method An alternative method has been proposed by Hansbo and Hansbo [35], in which two overlapping elements are introduced with independent displacement fields which are partially active. Cohesive tractions were applied in this method by Mergheim et al. [83], after which Song et al. [114] proved it to be equivalent to partition of unity enrichment with a discontinuous function and coined the term phantom node method.

An advantage of the phantom node method over traditional PUFEM is that the implementation is simpler, because it is not necessary to apply any changes to the elements adjacent to the cracked elements. Moreover, in dynamic methods, the phantom node method allows for straightforward lumping of the mass matrix in contrast with PUFEM. However, there is no similar extension to enrichment with asymptotic functions to approximate the singular stress field around the crack tip. Therefore, for modeling of cohesive cracking the phantom node method is to be preferred, while
Figure 1.6 Connectivity and active parts of two overlapping elements in phantom node method

for modeling of crack propagation in a fracture mechanics approach, PUFEM is the better alternative.

The phantom node method is illustrated in Figure 1.6. An element with original nodes \( n_1 \ldots n_4 \) is crossed by a crack at \( \Gamma_c \), dividing the element domain into two complementary sub-domains, \( \Omega_A \) and \( \Omega_B \). Phantom nodes (labeled \( \tilde{n}_1 \ldots \tilde{n}_4 \)) are added on top of the existing nodes. The existing element is replaced by two new elements, referred to as element \( A \) and element \( B \). The connectivity of these overlapping elements is

\[
\begin{align*}
\text{nodes}_A &= [\tilde{n}_1, \tilde{n}_2, n_3, n_4] \\
\text{nodes}_B &= [n_1, n_2, \tilde{n}_3, \tilde{n}_4]
\end{align*}
\]

(1.24)

The elements do not share nodes, and therefore have independent displacement fields. Both elements are only partially active, the active part of element \( A \) is \( \Omega_A \) and the active part of element \( B \) is \( \Omega_B \). This is represented numerically in the definition of the displacement field: the displacement of a point with coordinates \( x \) is computed with the standard finite element shape functions \( N(x) \) and the nodal displacement values from either of the overlapping elements, depending on the location of the point:

\[
\mathbf{u}(x) = \begin{cases} 
N(x) \mathbf{u}_A, & x \in \Omega_A \\
N(x) \mathbf{u}_B, & x \in \Omega_B 
\end{cases}
\]

(1.25)

The displacement jump over the crack is defined as the difference between the displacement fields of the two elements.

\[
[\mathbf{u}](x) = N(x) (\mathbf{u}_A - \mathbf{u}_B), \quad x \in \Gamma_c
\]

(1.26)

When this definition of the displacement field is combined with constitutive laws for the bulk stress and the cohesive traction, it follows from standard variational principles that the contribution to the internal force vector on the degrees of freedom
corresponding with element $A$ and $B$ are defined as

$$
f_A^{\text{int}} = \int_{\Omega_A} B^T \sigma \, d\Omega + \int_{\Gamma_c} N_t \, d\Gamma \quad (1.27)
$$

and

$$
f_B^{\text{int}} = \int_{\Omega_B} B^T \sigma \, d\Omega - \int_{\Gamma_c} N_t \, d\Gamma \quad (1.28)
$$

Because $f_A^{\text{int}}$ is coupled to $u_B$ (and $f_B^{\text{int}}$ to $u_A$) via $t(u)$ and Equation (1.26), the linearization also involves cross terms and the total contribution to the global tangent matrix is

$$
K = \begin{bmatrix}
K_A & 0 \\
0 & K_B
\end{bmatrix} + \begin{bmatrix}
K[u] & -K[u] \\
-K[u] & K[u]
\end{bmatrix} \quad (1.29)
$$

with

$$
K_I = \int_{\Omega_I} B^T D B \, d\Omega, \quad I = A, B \quad (1.30)
$$

$$
K[u] = \int_{\Gamma_c} N^T T N \, d\Gamma \quad (1.31)
$$

Because the law for the normal component is typically different from that for the shear component(s), transformations from the global coordinate frame to an orthonormal frame that is aligned with the crack (see Figure 1.6) and back are wrapped around the evaluation of the constitutive law. The displacement jump in local $\{n, s, t\}$-frame is related to the displacement jump in global $\{x, y, z\}$-frame with

$$
[u] = R[u] \quad (1.32)
$$

where, with $t$-axis parallel to the $z$-axis, the transformation matrix $R$ is given as

$$
R = \begin{bmatrix}
-\sin \phi & \cos \phi & 0 \\
\cos \phi & \sin \phi & 0 \\
0 & 0 & 1
\end{bmatrix} \quad (1.33)
$$

Similarly we have

$$
t = R t \quad (1.34)
$$

and (with $R^{-1} = R^T$)

$$
T = R^T T R \quad (1.35)
$$
1.4.3 Material parameters

Whether the description of choice is a continuum model with a stress-strain relation, or a discontinuous model with a traction-separation relation, in either case a constitutive law is needed, which is supposed to characterize the fracture behavior of the material. In formulating the constitutive law, a choice has to be made for the fundamental parameters. Ideally, the model contains only parameters that can be obtained from simple experiments and that are objective material constants. A common choice is to use strength and fracture energy. The strength of the material is the maximum stress the material can sustain, which is the peak level of the stress in Figure 1.3, while the fracture energy is the amount of energy that is required to form a unit area of new crack surface, which is related to the area under the curves in Figure 1.3. In a traction-separation law, the fracture energy is equal to the area under the curve, but in a stress-strain relation, the area under the curve is of the dimension energy per volume and has to be multiplied with the width of the failure zone in order to obtain the fracture energy.

In fracture mechanics, distinction is made between mode I (opening), mode II (in-plane shear) and mode III (out-of-plane shear), each of which is associated with a distinct value for the fracture energy. In computational practice, it is hard to distinguish between mode II and mode III and therefore a single shear mode is often utilized.

When uniaxial strength and pure mode fracture energy are determined, more assumptions and/or parameters are needed to interpolate for general stress state. In general stress space, strength becomes an envelope around the admissible stress states. And for general mixed mode fracture, the fracture energy becomes a function of the mode ratio.

In an idealized homogeneous material, strength and fracture energy can be related to fundamental bond forces on the nanolevel. In a heterogeneous material, however, the strength is dominated by irregularities in the microstructure. The failure load measured in a simple experiment is governed by stress concentrations due to stiffness inhomogeneity and/or triggered by spatial variation of the strength due to the presence of weak spots. Therefore size effects may play a role [6, 135]. Similarly, the fracture energy in a heterogeneous material is supposed to lump everything that is happening in the fracture process zone. However, it is debatable whether the energy dissipation in this zone is constant irrespective of geometry and the stress state around the tip. Indeed, evidence has been found that the fracture energy is not constant for composite materials [134].

Although doubts exist on the validity of these parameters, we follow the major part of the literature on composite materials and assume strength and fracture energy to be constant. Validation on a wide range of tests is needed to assert these assumptions.
But before such validation is possible, a framework must be developed that is generic and robust enough to work on such a wide range.

### 1.5 Mechanics of orthotropic materials

After the brief introduction of the numerical methods that are foundational for this work, we now pick up another trail, that of mechanics of composite materials. We focus on the mesolevel approach, which means that the unidirectional ply is considered a homogeneous material with orthotropic stiffness properties, i.e. a material that is more stiff in fiber direction than in transverse direction. Before failure, elastic properties can be scaled up fairly well to equivalent laminate properties with the classical lamination theory [47], or higher order theories [104]. This up-scaling allows for macroscale laminate analysis. However, in the failure process, the classical lamination theory or indeed any through thickness homogenization loses validity, particularly when delamination occurs and the displacement field of the different plies is no longer conforming.

**Elasticity** The starting point for the constitutive modeling is the law for elastic behavior of the elementary ply. Considering the fact that the ply is stiff in fiber direction and compliant in other directions, the transversely isotropic version of Hooke’s law is utilized, which is defined as

\[
\sigma = D^e \varepsilon
\]  

(1.36)

where \(E_1\) and \(E_2\) are the Young’s moduli of the ply in fiber direction and transverse direction respectively, \(\nu_{21}\) and \(\nu_{23}\) are the longitudinal and transverse Poisson’s ratios, and \(G_{12}\) is the longitudinal shear modulus. Under the assumption of transverse isotropy, the transverse shear modulus \(G_{23}\) is a dependent quantity, defined as:

\[
G_{23} = \frac{E_2}{2(1 + \nu_{23})}
\]  

(1.38)

The overbars in Equation (1.36) are used to indicate that the quantities are defined in the local material frame. In this frame, the 1-axis is aligned with the fiber direction.
in the ply, as illustrated in Figure 1.7. In this work only flat geometries are used where the local 3-axis is aligned with the global z-axis. Note that the fiber direction is indicated with $\theta$ in Figure 1.7.

**Transformations** In the finite element framework, stress and strain are defined in the global coordinate frame. This means that transformations are to be performed between the different frames. For a counterclockwise rotation (see Figure 1.7), the transformation of global stress vector $\bar{\sigma} = \{\sigma_x, \sigma_y, \sigma_z, \tau_{yz}, \tau_{zx}, \tau_{xy}\}$ to material stress vector $\bar{\sigma} = \{\sigma_1, \sigma_2, \sigma_3, \tau_{23}, \tau_{31}, \tau_{12}\}$ is defined as [47]

$$\bar{\sigma} = T \sigma$$  \hspace{1cm} (1.39)

with

$$T = \begin{bmatrix}
\cos^2 \theta & \sin^2 \theta & 0 & 0 & 0 & 2 \sin \theta \cos \theta \\
\sin^2 \theta & \cos^2 \theta & 0 & 0 & 0 & -2 \sin \theta \cos \theta \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & \cos \theta & - \sin \theta & 0 \\
0 & 0 & 0 & \sin \theta & \cos \theta & 0 \\
- \sin \theta \cos \theta & \sin \theta \cos \theta & 0 & 0 & 0 & \cos^2 \theta - \sin^2 \theta
\end{bmatrix}$$  \hspace{1cm} (1.40)

For strain transformation (when engineering strain is used with $\gamma_{12} = 2\varepsilon_{12}$) when the multiplications with the factor 2 are taken into account, it turns out that the transformation matrix is the transpose of the inverse of the transformation matrix for stress, i.e.:

$$\varepsilon = T^{-T} \varepsilon$$  \hspace{1cm} (1.41)

As long as the constitutive law is linear, it is computationally efficient to perform the transformation on the elastic stiffness matrix $D^e = T^{-1}D^eT^{-T}$ and update the stress directly in the global frame with $\sigma = D^e\varepsilon$, i.e.

$$\varepsilon \xrightarrow{\text{transformed constitutive law}} \sigma, D$$  \hspace{1cm} (1.42)
However, when a nonlinear law is defined in the material frame, it is necessary to perform the update of stress and tangent in the material frame and wrap it in transformation operations:

\[
\varepsilon \xrightarrow{\text{transformation}} \bar{\varepsilon} \xrightarrow{\text{constitutive law}} \bar{\sigma}, \bar{D} \xrightarrow{\text{transformation}^{-1}} \sigma, D \quad (1.43)
\]

**Residual stress**  An important aspect of laminate analysis is the residual stress due to fabrication. The difference in thermal properties of fiber and matrix causes the thermal expansion behavior of the ply to be orthotropic. When the laminate is cooled during fabrication, the plies will tend to shrink in transverse direction, but, since they are connected, this contraction is constrained. The transverse tensile stress that is caused by the mismatch in thermal properties can be significant with respect to the transverse tensile strength of the ply. Therefore it is important to take these residual stresses into account. For plane stress, the linear elastic constitutive law after a temperature change is

\[
\sigma = D\varepsilon^{\text{mech}} \quad (1.44)
\]

where the total strain is decomposed into a mechanical part and a thermal part:

\[
\varepsilon^{\text{mech}} = \bar{\varepsilon} - \varepsilon^{\text{th}} \quad (1.45)
\]

with

\[
\varepsilon^{\text{th}} = \{\alpha_1 \Delta T, \alpha_2 \Delta T, \alpha_2 \Delta T, 0, 0, 0\}^T \quad (1.46)
\]

where \(\Delta T\) is the magnitude of the change in temperature and \(\alpha_1\) and \(\alpha_2\) are the coefficients of thermal expansion in fiber direction and transverse direction, respectively.

1.6 Laminate failure analysis

This introductory chapter will be concluded with an overview of the state of the art in laminate failure analysis. Notable computational work has been done on the microlevel by González and LLorca [27], which illustrates the complexity of the mechanisms on that level. The need to incorporate the microlevel failure mechanisms in a multiscale framework is often stressed [40, 19, 74, 107]. To meet this need, sequential multiscale models for composite materials have been developed by Trias et al. [119], Drago and Pindera [24] and Ernst et al. [25], but for fully coupled multiscale failure analysis, more fundamental issues are yet to be resolved [92]. Moreover, good tools for monoscale mesolevel analysis will remain useful and the development of those is not yet completed.
1.6.1 Ply failure

A first step towards the analysis of laminate failure is the prediction of ply failure. The composite nature of the ply complicates the formulation of a stress based failure criterion. Unidirectional strength properties are measured for the characterization of the material, but in failure analysis, these have to be interpolated in order to get a general failure criterion (or set of criteria) to evaluate any three dimensional stress state for failure. Early work in the development of an orthotropic failure envelope was done by Hill [42], Tsai [120] and Hoffman [45]. Criteria were formulated, which consisted of a single relation for the interaction of the different stress components in the material frame. For composite materials, the most popular version of these so called interactive criteria is the one formulated by Tsai and Wu [121].

However, a single interactive criterion might just not reflect the level of complexity that is inherent in composite materials. A smooth failure envelope does not match the fact that, due to the inhomogeneity of the material, discrete switches from one type of failure to another are involved. Therefore, failure-mode-based theories have been proposed, with a number of independent criteria corresponding to an equal number of failure modes. The first failure theories that distinguished between fiber failure and matrix failure were developed by Hashin and Rotem [41, 40]. Many different formulations have been suggested since, among which the theories by Puck and Schürmann [102] and Dávila et al. [21, 98] are noteworthy.

The World Wide Failure Exercise organized by Hinton et al. (see [44, 113] and references therein) did not settle the case. A trade-off between accuracy of the criterion and the number of material parameters or assumptions involved will remain there, considering the fact that “a criterion is only as good as the data available”[68]. A problem with the failure criterion approach is that it is based on homogeneous stress while, as soon as failure starts somewhere in the specimen, stress is not homogeneous anymore. Size effects do play a role, which blurs the meaning of the concept of strength.

Furthermore, the statistical size effect is of importance for the phenomenon of fiber failure. The unidirectional ply strength in fiber direction is best described with a weakest link theory and a statistical distribution of the strength [135]. Numerous models have been developed to predict the ply strength in fiber direction as a function of the specimen size [36, 93, 53]. This issue will be left out of consideration in the modeling work in this thesis, because the concept of statistical strength distribution is at odds with the preference to build models that give a unique result.

Another complicating factor is that ply failure can be influenced by the presence of neighboring plies when the ply is embedded in a laminate. The neighboring plies have a constraining effect on the failure which makes it uncertain to what extent the failure can be characterized accurately with properties measured for the isolated ply.
A well-known example of this is the increase in transverse strength upon decreasing ply thickness, first reported by Parviz et al. [95]. Theories exist to predict the in situ strength. The relations proposed by Camanho et al. [14], for example, are incorporated in the failure criteria by Dávila et al. [21].

1.6.2 Progressive laminate failure

However, even if an accurate general failure criterion for the elementary ply could be formulated, this would not be sufficient for the prediction of laminate failure. One can use it to assess laminate failure in a First Ply Failure approach (see e.g. Schuecker et al. [111]), equating failure of a single ply to failure of the laminate, but in general, local failure of a ply does not necessarily lead to global laminate failure. Redistribution of stress may be possible such that the structure can be loaded beyond the load level at which first local failure occurs. In that case, in order to predict the load bearing capacity of a structure or structural part under specific load conditions, progressive failure analysis is required. That is, the failure criteria must be extended with a theory on what happens after failure.

The most simple approach to progressive failure analysis is the ply discount method. In this method the stiffness of a ply is reduced after the failure criterion is violated. This has been applied to matrix failure by Laš and Zemčík [60] and Liu et al. [67], and similarly to fiber failure by Li et al. [64]. These models, however, give mesh-dependent results. As long as the failure is triggered by the local stress, the amount of energy that is dissipated when a crack is formed vanishes upon mesh refinement. With a nonlocal failure criterion as by Li et al. [64] the mesh dependency is at least still present in a mesh size dependent amount of elastic energy that is discarded from the system upon crack growth.

In order to obtain a unique response, models with a continuous constitutive relation must be used. For orthotropic materials, several examples are available for extension of a failure criterion with a plasticity law [127, 62, 10, 69, 39]. But in the context of composite materials, continuum damage formulations are increasingly popular. After pioneering work by Ladévéze and Le Dantec [56] and Matzenmiller et al. [73], several different formulations have been proposed in which distinction is made between fiber failure and matrix failure [55, 70, 59, 58, 16, 26, 100, 101]. These are more easily coupled to the failure-mode-based criteria, with different stiffness degradation laws for the different failure processes.

1.6.3 Delamination

From micromechanical point of view, damage between the plies is matrix failure. In full three-dimensional analysis, therefore, it makes sense to use the same model for transverse matrix cracking and delamination. This has been done by Maimi et
al. [72]. However, because of the particular orientation of delamination cracks, it pays off to give them a separate treatment. A continuum approach to delamination requires a considerable fineness of discretization through the thickness of the laminates, which can be avoided when the interface between the plies is modeled with interface elements.

Modeling of delamination with interface elements was first done by Schellekens and De Borst [110] and Allix and Ladevèze [2]. Schellekens and De Borst developed a plasticity formulation which was further pursued by Hashagen and De Borst [38]. However, robustness and ease of implementation renders damage formulations favorable. Besides, when a delamination crack propagates, it does not make much difference whether deformations in the process zone are considered permanent or not. A simple bilinear softening law for mixed mode failure was proposed by Mi et al. [85]. Camanho et al. [13] developed a law in which the fracture energy is a phenomenological function of the mode mixity as formulated by Benzegagh and Kenane [9]. This formulation was improved for thermodynamical consistency by Turon et al. [122] and again for a consistent formulation under varying mode ratio [123]. Alternative formulations have been proposed among others by Jiang et al. [50] and Yang and Cox [139]. Generally, these damage laws have a simple dummy stiffness to prevent interpenetration and allow for compressive forces to be transmitted through the interface. What is not taken into account, however, is the possibility of a significant increase in strength and mode II fracture energy in the presence of compressive stress. This issue has been addressed by Li et al. [63]. Even in the absence of compressive stress, the fracture energy is not always constant, as has been observed by Wisnom [134].

The partition of unity method has been applied to delamination problems by Wells et al. for volume elements [131] and solid-like shell elements [106]. The advantage of the partition of unity method is that the problem size is kept as low as possible because additional degrees of freedom are inserted only where cracking is eventuated. For modeling of delamination, however, the particular advantage of interface elements over the partition of unity method is that initiation of new cracks can be taken care of in a straightforward manner with the elastic tractions that are already present before there is a crack. This advantage even holds for the propagation of cracks, because tractions in interface elements sooner tend to offer an accurate estimate of the interface tractions than the volume stresses in continuum elements, which require a rather fine discretization.

1.6.4 Complete analysis

Eventually, constitutive models will have to prove their value in complete analyses where different processes may occur and interact. However, examples of complete
progressive failure analyses are sparsely found. Good examples of the application of continuum damage models for cases without delamination have been presented by Camanho et al. [16, 15] and Blom et al. [11]. The mentioned paper by Maimi et al. [72] shows good results from three dimensional analyses involving matrix cracking in 90°-plies in interaction with delamination and ending up in fiber failure. Notable success in representing subcritical damage (matrix cracking and delamination) around a notch with a simple ply discount method was reported by Liu et al. [67].

An alternative strategy is built around the idea to model matrix cracks by inserting interface elements through the thickness of the ply at selected locations. This strategy, first employed by Wisnom and Chang [136], gives good interaction with interface elements for delamination. Similar work has been done by De Moura and Gonçalves [23] and Yang and Cox [139]. Wisnom, Hallett and coworkers have further applied this on different notched and unnotched geometries with considerable success [34, 50, 33]. Subsequently, a Weibull criterion was added to predict brittle fiber failure [32], which was later applied to cases with progressive fiber failure [64].

The objective of the work presented in this thesis is to build a numerical framework that allows for predictive modeling of complex failure mechanisms with matrix cracking, delamination and fiber failure.
Chapter 2 Constitutive ply modeling

This chapter deals with the modeling of failure of a single unidirectional ply. The intact ply is modeled as an orthotropic elastic material, which is stiff in fiber direction and relatively weak in transverse directions. This model must be extended with descriptions for the different failure processes and the question is how this can be done in a realistic manner. Failure criteria are needed as well as laws that describe what happens after a failure criterion is violated.

In Section 2.1, the possibility to use continuum modeling as a generic framework for all ply failure mechanisms is examined, and it is concluded that this is not the way to go. This is a pivotal observation for this dissertation, since it provides the motivation to use the phantom node method for matrix cracking, which forms the basis for the proposed framework. In Section 2.2 application of the phantom node method is proposed as a better approach to the modeling of matrix cracking. For this specific application, difficulties are encountered in the formulation of the cohesive law. Two different cohesive laws in which these difficulties are avoided are presented in Section 2.3 and 2.4. Next, two continuum models are presented that can be combined with the discontinuous representation of matrix cracking in order to end up with a complete description of the ply behavior. The first, in Section 2.5, deals with fiber failure, and the second, in Section 2.6, with shear nonlinearity.

For simplicity of notation, thermal strain and coordinate frame transformations are left out of consideration in the treatment of constitutive laws in this chapter. In the implementation, the bulk constitutive laws are wrapped in transformations and preceded by subtraction of thermal strain (see Section 1.5), and the cohesive laws are wrapped in transformations from the global coordinate frame to the local frame on the crack surface (see Section 1.4.2).

2.1 Continuum models and their limitation

In this section, two different continuum models for ply failure will be presented and it will be shown in a simple numerical example how both fail in representing matrix failure properly. The two models are specifically designed to describe failure behavior of unidirectional composites, taking into account the fact that the strength properties are orthotropic, viz. that the material is strong in fiber direction and weak in transverse direction. In both cases, viscous regularization is applied to ensure the mesh-independence of the numerical response.
Discrete crack

Damaged band

\( \gamma_{12} \)

\( \tau_{12} \)

(a) (b) (c)

Figure 2.1 Micromechanical representation of matrix failure oriented in fiber direction (a) and matrix failure in a band crossed by fibers (b). The difference in averaged stress-strain response is illustrated schematically (c).

There is a pathology in the continuum approach, which can be understood from simple micromechanical considerations. When looking at the micromechanical failure process, the orientation of a band with matrix failure influences its effect on the composite. A band with shear failure that is oriented in fiber direction can develop into a macrocrack running between the fibers, which is a relatively brittle mechanism, while a band with matrix shear failure in any other direction is crossed by fibers, and the corresponding failure mechanism is therefore more ductile (see Figure 2.1). In continuum models, however, this distinction cannot be made. In the homogenized continuum, both mechanisms are represented with a softening shear band with the same local stress-strain relation.

2.1.1 Softening plasticity

Firstly, a softening plasticity model is presented. The general idea behind plasticity has been introduced in Section 1.4.1, here it is applied in the context of orthotropic materials.

Failure criterion Because of the complexity and possible instability of the stress evaluation in the plasticity approach, a single expression failure criterion is preferable. Therefore, the Tsai-Wu criterion [121] is adopted, which can be written as:

\[
f(\sigma) = \frac{1}{2} \sigma^T P^0 \sigma + \sigma^T p^0 - 1 = 0
\]  

where matrix \( P^0 \) and vector \( p^0 \) are computed from orthotropic uniaxial strength parameters (cf. [108]). These are the tensile and compressive strength in fiber direction, \( F_{1t} \) and \( F_{1c} \), the tensile and compressive transverse strength \( F_{2t} \) and \( F_{2c} \), and the longitudinal and transverse shear strength \( F_{12} \) and \( F_{23} \).
Softening is introduced by shrinking the yield surface \( f = 0 \) as the plastic strain grows. For sake of simplicity, linear isotropic softening is adopted; isotropic in the sense that all uniaxial strength parameters are multiplied with the same factor \( h(\kappa) \), where \( \kappa \) is a state variable. Initially \( h = 1 \) and when \( h = 0.01 \) the material is considered to have failed. As such the yield function becomes a function of \( \kappa \) which may be written as:

\[
f(\sigma, \kappa) = \frac{1}{2} \sigma^T P(\kappa) \sigma + \sigma^T p(\kappa) - 1 = 0 \tag{2.2}
\]

with

\[
P(\kappa) = \frac{1}{h(\kappa)^2} p^0, \quad p(\kappa) = \frac{1}{h(\kappa)} p^0 \tag{2.3}
\]

**Plastic strain evolution** The plastic strain \( \varepsilon^p \) (see Equation (1.14)) grows whenever that is necessary to ensure that the criterion \( f(\sigma, \kappa) \leq 0 \) is satisfied. The plastic strain rate is given by

\[
\dot{\varepsilon}^p = \dot{\lambda} m \tag{2.4}
\]

where \( m \) is the direction of plastic strain, which is, under the assumption of associative flow, defined as

\[
m = \frac{\partial f}{\partial \sigma} \tag{2.5}
\]

The evolution of plastic multiplier \( \dot{\lambda} \) is such that the Kuhn-Tucker conditions are satisfied:

\[
f \leq 0, \quad \dot{\lambda} \geq 0, \quad f \dot{\lambda} = 0 \tag{2.6}
\]

For regularization, the consistency model by Wang et al. [130] is applied by inserting a rate dependent term in the evolution law for \( h \):

\[
h(\kappa, \dot{\kappa}) = 1 - S \kappa + V \dot{\kappa} \tag{2.7}
\]

where \( S \) is the softening parameter and \( V \) the viscosity parameter (see Figure 2.2).

The model formulation is completed with an evolution law for state variable \( \kappa \), which is defined as

\[
\dot{\kappa} = \frac{1}{h} \sigma_i Q_i \varepsilon^p_i \tag{2.8}
\]

in which \( Q_1 = 1 \) and the other parameters \( Q_i, i = 2 \ldots 6 \) may be tuned in order to control the energy dissipated in a uniaxial case independently for each loading direction. Via Equation (2.4), \( \dot{\kappa} \) is related to \( \dot{\lambda} \). A return mapping algorithm has been designed to find the values of the fundamental unknowns in the constitutive relation, \( \sigma \) and \( \Delta \lambda \), for which the basic equations, Equation (1.14) and Equation (2.2), are satisfied.
Chapter 2 Constitutive ply modeling

Rate independent strength: \((1 - S\kappa)F_{1t}\)

Figure 2.2 Schematic representation of uniaxial stress-strain relation with softening visco-plasticity.

**Linearization** For the sake of robustness, care is required in the derivation of the consistent tangent. The consistent tangent is given by:

\[
D = H - \frac{Hmn^T H}{\mu + n^T Hm} \tag{2.9}
\]

with

\[
n = m + \frac{\partial f}{\partial \kappa} \left( \frac{\partial \kappa}{\partial m} \right)^T E^{-1} P \tag{2.10}
\]

\[
\mu = -\frac{\partial f}{\partial \kappa} \frac{\partial \kappa}{\partial \lambda} \left( 1 + \left( \frac{\partial \kappa}{\partial m} \right)^T E^{-1} \frac{\partial m}{\partial \kappa} \right) \tag{2.11}
\]

\[
H = \left[ I + \Delta \lambda D^e E^{-1} P \right]^{-1} D^e \tag{2.12}
\]

\[
m = m + \Delta \lambda E^{-1} \frac{\partial m}{\partial \kappa} \frac{\partial \kappa}{\partial \lambda} \tag{2.13}
\]

where \(\Delta \lambda\) is the finite increment of the plastic multiplier for the current time step and

\[
E = I - \frac{\partial m}{\partial \kappa} \left( \frac{\partial \kappa}{\partial m} \right)^T \tag{2.14}
\]

Upon unloading \((f < 0 \Rightarrow \dot{\lambda} = 0)\), the consistent tangent reduces to the initial elastic stiffness \(D^e\).

**2.1.2 Continuum damage**

As an alternative to the softening plasticity model, a continuum damage model for the homogenized unidirectional ply is presented. This formulation is similar to several models that have been introduced in literature (see e.g. [73, 101, 59, 70, 71, 58]).
2.1 Continuum models and their limitation

Stress update

Orthotropic stiffness degradation is accomplished by using two independent damage variables, one related to fiber failure and the other related to matrix failure. Following Matzenmiller et al. [73], damage is taken into account via modification of the values on the diagonal of the compliance matrix, such that the constitutive law is defined as

\[ \sigma = C^{-1} \varepsilon \quad (2.15) \]

with

\[
C = \begin{bmatrix}
\frac{1}{(1-\omega_f)E_1} & -\frac{\nu_{21}}{E_2} & -\frac{\nu_{23}}{E_2} & 0 & 0 & 0 \\
-\frac{\nu_{21}}{E_2} & \frac{1}{(1-\omega_m)E_2} & -\frac{\nu_{23}}{E_2} & 0 & 0 & 0 \\
-\frac{\nu_{23}}{E_2} & -\frac{\nu_{21}}{E_2} & \frac{1}{(1-\omega_m)E_2} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{(1-\omega_m)G_{12}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{(1-\omega_m)G_{23}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{(1-\omega_m)G_{12}}
\end{bmatrix} \quad (2.16)
\]

where \( \omega_f \) and \( \omega_m \) are the damage variables related to fiber failure and matrix failure, respectively.

Damage evolution

With separate variables for matrix damage and fiber damage, it is logical to use failure-mode-based failure criteria for initiation and evolution of damage. For the damage evolution these criteria evaluate the effective stress, which can be understood as the stress acting on the intact material:

\[ \sigma_{\text{eff}} = D^c \varepsilon \quad (2.17) \]

Hashin’s failure criteria [41, 40] are selected for their relative simplicity. Four criteria are distinguished:

Tensile fiber mode:

\[ f_{\text{ft}} = \frac{\sigma_{\text{eff}}}{F_{1t}} \quad (2.18) \]

Compressive fiber mode:

\[ f_{\text{fc}} = -\frac{\sigma_{\text{eff}}}{F_{1c}} \quad (2.19) \]

Tensile matrix mode:

\[ f_{\text{mt}} = \sqrt{\left(\frac{\sigma_{\text{eff}}}{F_{2t}}\right)^2 + \left(\frac{\tau_{\text{eff}}}{F_{23}}\right)^2} \quad (2.20) \]
Compressive matrix mode:

\[
f_{mc} = \sqrt{\left(\frac{F_{2c}}{F_{23}}\right)^2 - 1} \frac{\sigma_{eff}^2 + \sigma_{eff}^3}{\sigma_{eff}^2 + \sigma_{eff}^3} + \frac{(\sigma_{eff}^2 + \sigma_{eff}^3)^2}{4F_{23}} + \frac{(\sigma_{eff}^2 - \sigma_{eff}^3)^2}{F_{23}} + \frac{(\tau_{eff}^2)^2 + (\tau_{eff}^3)^2}{F_{12}}
\]

where \(F_{1t}\) and \(F_{1c}\) are the tensile and compressive strength in fiber direction, \(F_{2t}\) and \(F_{2c}\) are the tensile and compressive transverse strength, and \(F_{23}\) and \(F_{12}\) are the transverse and longitudinal shear strength.

With the failure criteria, two loading functions \(\phi_i\) are evaluated, one corresponding to fiber failure and the other to matrix failure

\[
\phi_i = \begin{cases} 
  f_{ft}, & \sigma_{eff}^1 \geq 0 \\
  f_{fc}, & \sigma_{eff}^1 < 0 
\end{cases}
\]

\[
\phi_m = \begin{cases} 
  f_{mt}, & \sigma_{eff}^2 + \sigma_{eff}^3 \geq 0 \\
  f_{mc}, & \sigma_{eff}^2 + \sigma_{eff}^3 < 0 
\end{cases}
\]

For both fiber and matrix failure, there is a single state variable \(\kappa_i\). For simplicity, there is no distinction between compressive and tensile failure regarding the state of the material. An artificial viscosity, limiting the rate of state variable \(\kappa_i\), is introduced for regularization, such that the evolution of \(\kappa_i\) is defined as (cf. \[54, 1, 140\])

\[
\dot{\kappa}_i = B_i \langle 1 - \phi_i - \kappa_i \rangle, \quad i = f, m
\]

where \(B_i\) is the maximum rate with which \(\kappa_i\) is allowed to increase and the operator \(\langle x \rangle = (x + |x|)/2\) is used to ensure irreversibility of the damage process. In the rate independent limit \(B_i \to \infty\), Equation (2.24) reduces to \(\kappa_i = \sup(\phi_i - 1)\).

Damage variables \(\omega_i\) are computed from \(\kappa_i\) according to

\[
\omega_i = \min \left\{ 1, \frac{A_i \kappa_i}{(\kappa_i + 1)(A_i - 1)} \right\}, \quad i = f, m
\]

which corresponds to a bilinear stress-strain relation for uniaxial tests without viscosity. The softening parameter \(A_i\) is related to the strain level at which complete failure occurs in this bilinear relation (see Figure 2.3), and hence to the fracture energy, although the actual amount of dissipated energy is rate-dependent.

**Linearization** The consistent tangent is obtained by taking an infinitesimal variation of the constitutive law (2.15) with respect to both stress and strain. The ratio between the stress increment and the strain increment can be written as

\[
D = C^{-1} [I - M]
\]
2.1 Continuum models and their limitation

\[ M_{ij} = \sigma_i \frac{\partial C_{ii}}{\partial \omega_k} \frac{\partial \omega_k}{\partial \phi_k} \frac{\partial \phi_k}{\partial \varepsilon_j}, \quad k = f, m \]  

Upon unloading the consistent stiffness matrix reduces to the secant stiffness \( C^{-1} \).

### 2.1.3 Off-axis tensile test

To illustrate the pathology of continuum models with respect to matrix crack simulation, a uniaxial tensile test on a 10° unidirectional laminate is considered. This is a standard test for the determination of the in-plane shear strength [18, 125]. The test is performed on a specimen with the shape of a parallelogram, as shown in Figure 2.4, where the oblique ends are used to remove stress concentrations from the boundaries. Experiments show brittle matrix failure. In a sudden event, the specimen breaks, with the crack running in fiber direction.

A displacement in \( x \)-direction is applied to the right side of the specimen, which is free in \( y \)-direction. Oblique ends with an angle of 54° with the load direction are used, so that for linear elasticity the stress state is homogeneous, thus eliminating edge effects. The material parameters are summarized in Table 2.1. In order to trigger localization the longitudinal shear strength \( F_{12} \) is reduced from 52 to 40 MPa in an area of 1 × 0.5 mm. Two different meshes are used, with respective in-plane element sizes of 0.5 × 0.5 mm and 0.25 × 0.25 mm in the area of interest.

![Figure 2.3](image1.png)  

**Figure 2.3** Schematic representation of uniaxial stress-strain relation for continuum damage with artificial viscosity.

![Figure 2.4](image2.png)  

**Figure 2.4** Off-axis tensile test: geometry and experimentally observed crack path.
Table 2.1 Material parameters for off-axis tensile test. Elasticity and tensile strength parameters are taken from Van Paepegem et al. [125] (glass/epoxy).

<table>
<thead>
<tr>
<th>Elasticity</th>
<th>Ply strength</th>
<th>Plasticity</th>
<th>Damage</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$ 38.9 GPa</td>
<td>$F_{1t}$ 901 MPa</td>
<td>$S$ 10 MPa$^{-1}$</td>
<td>$A_f$ 100 s$^{-1}$</td>
</tr>
<tr>
<td>$E_2$ 13.3 GPa</td>
<td>$F_{1c}$ 800 MPa</td>
<td>$V$ 0.1 s/MPa</td>
<td>$A_{tm}$ 3 s$^{-1}$</td>
</tr>
<tr>
<td>$v_{21}$ 0.26</td>
<td>$F_{2t}$ 36.5 MPa</td>
<td>$Q_{2..6}$ 0.1</td>
<td>$B_f$ 60 s$^{-1}$</td>
</tr>
<tr>
<td>$v_{23}$ 0.4</td>
<td>$F_{2c}$ 70 MPa</td>
<td></td>
<td>$B_{tm}$ 60 s$^{-1}$</td>
</tr>
<tr>
<td>$G_{12}$ 5.13 GPa</td>
<td>$F_{12}$ 52 MPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$F_{23}$ 34.8 MPa</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 2.5 shows the load displacement diagram and final deformation obtained with the plasticity model and the damage model. The influence of the element size on the load-displacement behavior is negligible, which is related to the fact that the band with localized strain is wider than the elements, due to the viscous term. The deformed meshes, which are taken from the coarse mesh analyses, clearly show a failure pattern that is different from that observed in experiments. The failure band is not aligned with the fibers.

Notably, in both cases there is a significant displacement perpendicular to the load direction. The deformation in the localization area is such that the strain in fiber direction $\varepsilon_1$ remains relatively small. In the damage model, this is caused by the fact that the stiffness in fiber direction remains almost completely unaffected during the analysis. In the plasticity model, the same deformation is observed, in spite of the fact that the material degradation in that model is isotropic. Here it is caused
2.1 Continuum models and their limitation

by the flow rule, which ensures that the dominant direction of nonlinear strain is related to the direction in which the yield criterion is violated. Hence, both models give locally correct behavior, where a stress state for which the transverse strength is exceeded never gives rise to large strains in fiber direction.

However, although the local behavior is correct, the global behavior is not. The fact that $\varepsilon_1$ remains small, is not sufficient to ensure that matrix failure develops in fiber direction. The cause for this behavior lies in the fact that the direction of failure propagation in the model is governed by the stress concentration rather than by the fiber direction. This is a consequence of the homogenization which is fundamental to continuum models. In a homogenized model the smeared crack will always propagate there where the stress is highest, whereas in the real material the very fact that the material is inhomogeneous causes the crack to grow differently, as shown in Figure 2.6.

With this example, the consequences of the limitation of the continuum approach are clearly visible. It can be concluded that there is a fundamental problem in the modeling of failure in composites with continuum models. The micromechanical cause for cracks to grow in fiber direction, is not present in continuum models, at least not as long as the model descriptions are purely local. This can be considered a special case of violation of the principle of separation of scales. In Chapter 1, the microscale has been introduced as the level where individual fibers and the matrix material are distinctively present, while on the mesoscale, the material is homogenized. As such, an individual matrix crack is a typical microscale phenomenon. When it is brought to the mesoscale through homogenization it is no longer individually represented. In reality, however, an individual matrix crack may grow very large, and play a role on a higher scale. After homogenization in the micro-meso transition, this information is lost.

It is unlikely that mechanisms, in which large cracks in fiber direction play a role in different plies with different fiber orientations, can be predicted using state-of-the-art continuum models for ply failure, irrespective of the failure criteria and damage evolution laws that are applied. However, for other failure mechanisms, the continuum description might serve well, e.g. when failure in all plies is localized in a single plane [16]. In some cases the matrix crack will emerge correctly, such as the
45° crack presented by Pinho et al. [101], the split near a circular hole as reported by Cox and Yang [19] and the split in the 0°-ply in the notched plate example. But, as far as localized matrix failure in a single ply is concerned, the predictive quality of continuum models should be doubted.

2.2 A discontinuous approach to matrix cracking

On the mesolevel, where matrix and fibers are not modeled separately, it is necessary to enforce the orientation of the matrix cracks in order to describe the mechanisms realistically. This can be done by modeling matrix cracks with interface elements that are inserted in the mesh a priori as proposed by Wisnom et al. [136, 50, 32, 64]. However, this requires additional meshing effort and is less predictive because the possible crack locations have to be predefined. Therefore a mesh-independent representation of discontinuities, such as possible with the partition of unity finite element method (see Section 1.4.2), is to be preferred for the simulation of matrix cracking. Techniques for mesh-independent representation of discontinuities have been applied in the context of matrix cracking by Iarve et al. [48, 88] and Ling et al. [66].

Fundamental choices With partition of unity based methods, crack initiation and growth can be simulated at arbitrary locations in the mesh. For this, generally two criteria are needed, the first to judge whether the crack will grow and the second to determine in which direction the crack will grow. From this point of view, application of these methods to the simulation of matrix cracking in laminates is a simplification, for the second criterion becomes trivial: the direction of crack growth is always equal to the fiber direction. A matrix crack grows by definition between the fibers, and this can be numerically enforced by fixing the direction of crack growth ($\phi$ in Figure 1.6 is set equal to $\theta$ in Figure 1.7). As long as one layer of elements is used through the thickness of the ply, it is naturally assumed that matrix cracks always extend through the ply thickness. Because of this, complications in describing three dimensional crack paths (see e.g. [49]) are avoided in three dimensional analysis.

In this work, it is assumed that the matrix crack orientation is always perpendicular to the laminate plane. In plane stress analysis, this is inevitable, but in three-dimensional analysis, it is in principle possible to make the through thickness orientation variable. This could allow for modeling of the compressive failure mechanism in laminates due to the wedge effect on inclined matrix cracks [102]. In this thesis, however, only tensile load cases are considered, for which the assumption of vertical cracking is fair.

For the simulation of propagating matrix cracks, the cohesive approach is chosen over the brittle version with crack tip enhancement. In the first place because the
2.2 A discontinuous approach to matrix cracking

Cohesive tractions and hence a fine mesh are needed anyway for delamination when through thickness discretization is coarse. And secondly because it is not clear what the singular functions should look like for a crack tip in an orthotropic medium that is constrained by neighboring plies. As motivated in Section 1.4.2, with this choice the phantom node method is the preferred implementation.

In laminate analysis, distributed cracking may occur, which can also be handled with the phantom node method, although the number of cracks has to be limited. This will be treated in Section 3.3. The check for initiation and propagation of cracks occurs with a failure mechanism that is evaluated in all elements where cracking is allowed after convergence has been reached. The algorithmic treatment of the insertion of new crack segments will be given attention in Section 4.2.

**Cohesive laws** In contrast with interface elements, the phantom node method requires an initially rigid cohesive law, because the cohesive segments are introduced at nonzero stress level. In most texts on propagating cohesive cracks in partition of unity based formulations, decohesion is mode I driven, either by leaving out shear tractions altogether [86, 114, 103], or by assuming constant shear stiffness [83], or by assuming decreasing shear stiffness where the decrease is driven by normal crack opening only [132, 20]. This simplification is compatible with a crack propagation procedure that is based on direction of maximum principal stress, because then the shear traction is at least initially equal to zero. In the present case of matrix cracking, however, the crack propagation direction is independent of the stress field, and a complete mixed mode formulation is needed. However, such formulations are not readily available.

It is possible to define an initially rigid mixed mode damage law that computes the traction vector from the displacement jump (see e.g. Oliver [94] and Mergheim and Steinmann [84]). However, the traction is then not uniquely defined for zero crack opening (see Figure 2.7; all isolines for the traction go through $[u] = 0$). In a uniaxial case it is obvious that the traction should be equal to the strength. But in a mixed mode formulation the strength is a surface in the traction space and the initial traction can be any point on that surface. The traction evaluation itself remains feasible, because the crack opening after a finite load increment will not be exactly equal to zero. However, the highly nonlinear nature of the traction separation law around the origin endangers the stability of the Newton-Raphson procedure. Very small variations in nodal displacements give rise to large changes in nodal forces and also, more critically, to large changes in the tangent matrix, which leads to ill-convergence.

However, more knowledge on the initial traction is available. Namely, that the cohesive traction acting on the crack surface must be in equilibrium with the stress
Chapter 2 Constitutive ply modeling

Figure 2.7 Tractions in initially rigid mixed mode cohesive law. Each straight line corresponds with a fixed ratio $[u]_n/[u]_s$. The traction is not uniquely defined at $[u] = 0$.

in the bulk material next to the crack:

$$ t = \sigma n $$  \hspace{1cm} (2.28)

where $\sigma$ is the stress tensor and $n$ the normal vector of the crack surface. Notably, since the crack is parallel to the fiber, the vector $\sigma n$ contains the material stress components $\sigma_2$ and $\tau_{12}$. The value of $\sigma n$ upon crack initiation is known and can be used for the evaluation of the initial traction.

In this chapter, two laws that do this are introduced. In both cases, it is assumed that the fracture energy of the material can be described properly with the phenomenological relation proposed for delamination by Benzeggagh and Kenane [9], which has been applied in interface elements by [13] and [122]:

$$ G_{Tc} = G_{IC,m} + (G_{IIC,m} - G_{IC,m}) \alpha \eta $$  \hspace{1cm} (2.29)

in which $G_{IC,m}$ is the mode I fracture energy, $G_{IIC,m}$ is the mode II fracture energy, $\eta$ is a mode interaction parameter, and $\alpha$ is the ratio between the actual dissipation in the two modes, defined as:

$$ \alpha = \frac{G_{II}}{G_I + G_{II}} $$  \hspace{1cm} (2.30)

But before the cohesive laws are introduced, the off-axis tensile test from Section 2.1.3 is revisited to illustrate the suitability of the method.

Off-axis tensile test  As far as applicable, the material parameters from Table 2.1 are re-used. The fracture energy for the matrix cracks ($G_{IC,m} = G_{IIC,m}$) is set to
3.0 N/mm. The bulk constrained cohesive law that will be described in Section 2.3 is used. Notably, the geometry is such, that the stress field is homogeneous until nonlinearities occur, which means that the failure criterion is violated simultaneously in the whole specimen. To overcome the consequential non-uniqueness, the location of crack initiation is specified in advance (see Figure 2.4).

In Figure 2.8, it can be observed that the correct crack path is predicted. The deformed mesh is shown for three time steps, along with the corresponding load-displacement plots. In a sudden event at the peak load level, a cohesive crack of considerable length appears, after which the load drops in a sharp snapback without much additional crack growth. Then the cohesive zone, i.e. the part of the crack in which tractions are present, becomes smaller and the crack propagates toward the opposite boundary of the specimen. The crack grows in the correct direction. This is in itself not surprising, since the growth direction is predefined, but it is exactly this, that the direction of crack propagation can be fixed, which should in this context be considered a great advantage of the discontinuous approach in this context over continuum models (cf. Figure 2.5). Thus, the micromechanical phenomenon that
matrix cracks grow parallel to the fiber, is incorporated on the mesolevel.

Furthermore, in the final load-displacement diagram in Figure 2.8, the response is compared with that from a second analysis with a finer mesh. The averaged element size in the coarse mesh is $1.1 \times 0.5$ mm while that in the fine mesh is $0.8 \times 0.25$ mm. It can be observed that, in contrast with local continuum models for failure, mesh-independent results are obtained without special precautions. The snapback behavior is captured with the dissipation-based arclength method (see Section 4.1).

### 2.3 Bulk stress constrained cohesive law

As motivated above, an initially rigid mixed mode cohesive law needs to be formulated such that no singularity exists for zero damage and zero crack opening. The first law that satisfies this requirement is constructed by including the stress in the neighboring bulk material directly in the formulation using equilibrium considerations. This law is based on earlier work by Moonen et al. [89] and presented below in the local \{n, s, t\}-frame (see Figure 1.6).

**Failure criterion**  The cohesive law is related to the failure criterion that is used, because the stress level at which failure is initiated defines the initial traction for zero opening and zero damage. With this cohesive law, the test for propagation or initiation is performed with a simple interactive stress criterion (cf. [40]). A new crack segment is inserted when

$$\left(\frac{\langle \sigma_2 \rangle}{F_{2t}}\right)^2 + \left(\frac{\tau_{sh}}{F_{12}}\right)^2 > 1$$

(2.31)

in which $F_{2t}$ is the transverse tensile strength, $F_{12}$ is the longitudinal shear strength and $\tau_{sh}$ is the norm of the shear stress components acting on the vertical plane.

$$\tau_{sh}^2 = \tau_{12}^2 + \tau_{23}^2$$

(2.32)

Note that for 3D analyses it is assumed here that $F_{12} = F_{23}$.

**Traction update**  The starting point for the traction law is an initially rigid law [94], written as

$$t = \frac{1 - \omega_m}{\omega_m} T \llbracket u \rrbracket$$

(2.33)

in which $\omega_m$ is a damage variable that evolves from 0 to 1 during crack opening and $T$ is a stiffness parameter. In this formulation, the aforementioned non-uniqueness exists for $\omega_m = 0$ and $\llbracket u \rrbracket = 0$. Therefore the law is rewritten. First, Equation (2.33)
2.3 Bulk stress constrained cohesive law

is reformulated by multiplying with $\omega_m$ and adding $(1 - \omega_m)t$ on both sides, which gives:

$$t = (1 - \omega_m) \{ t + T[u] \}$$

(2.34)

Next, the equilibrium relation in Equation (2.28) is substituted in the right hand side of Equation (2.34):

$$t = (1 - \omega_m) \{ H\sigma + T[u] \}$$

(2.35)

where $H\sigma$ is the equivalent in Voigt notation for the contraction of the stress tensor with the normal vector $\sigma n$. With Equation (2.35), the traction is always uniquely defined. For zero damage and zero jump the traction is explicitly equal to $\sigma n$. The part between braces will be referred to as the effective traction, $t_{eff}$.

In order to prevent interpenetration of the cracked parts, the damage variable is replaced with a damage tensor. With this, the traction is defined as:

$$t = [I - \Omega]t_{eff}$$

(2.36)

with (in tensor notation)

$$\Omega_{ij} = \omega_m \delta_{ij} \left( 1 - \delta_{i1} \frac{t_{eff}^n}{t_{eff}^n} \right)$$

(2.37)

where $\delta_{ij}$ is the Kronecker delta. In words, Equations (2.36) and (2.37) signify that the damage is applied on all traction components, except on the normal component when the normal component of the effective traction is negative. This suffices to prevent interpenetration because with this factor, $t_{eff}^n < 0 \Rightarrow t_n = t_{eff}^n$, and, with the assumption of equilibrium ($t_n = \sigma_2$), this gives in turn $t_n = t_{eff}^n \Rightarrow \|u\|_n = 0$. Because equilibrium is only weakly met, limited interpenetration may occur, but this can be expected to vanish upon mesh refinement.

**Damage evolution** During the failure process, the effective traction increases. The damage evolution is driven by $\kappa_m$, which is a scalar measure for the magnitude of the effective traction:

$$\kappa_m = \sqrt{\left( \frac{t_{eff}^n}{F_{2n}} \right)^2 + \left( \frac{t_{eff}^{sh}}{F_{12}} \right)^2}$$

(2.38)

with

$$\left( t_{eff}^n \right)^2 = \left( t_{sh}^n \right)^2 + \left( t_{eff}^t \right)^2$$

(2.39)
This $\kappa_m$ is used for the evolution of damage variable $\omega_m$:

$$\omega_m = \max_{t \leq \tau} \begin{cases} \frac{\kappa_f^m(\kappa_m - 1)}{\kappa_m(\kappa_f^m - 1)}, & \kappa_m < \kappa_f^m \\ 1, & \kappa_m \geq \kappa_f^m \end{cases} \quad (2.40)$$

which results in a linear softening relation between traction and separation. The definition of $\kappa_m$ in Equation (2.38) is of the same form as the failure criterion in Equation (2.31), which is no coincidence. Upon crack initiation, $\kappa_m = 1$, which gives $\omega_m = 0$. As such, continuity in the response of the cracking element is ensured.

In Equation (2.40), the operator $\max_{t \leq \tau}$ ensures that the damage variable is monotonically increasing.

In the cracked element, the bulk stress at $\Gamma_c$, which is used in the evaluation of the effective traction, is not uniquely defined. The averaged strain from both overlapping elements is used:

$$\sigma = \sigma(\varepsilon_{\Gamma_c}) \quad (2.41)$$

with

$$\varepsilon_{\Gamma_c} = \frac{1}{2} (\varepsilon_{\Gamma_c^+} + \varepsilon_{\Gamma_c^-}) = \frac{1}{2} \mathbf{B}(x_{\Gamma_c}) (u_A + u_B) \quad (2.42)$$

It can be shown that for a fixed mode ratio, the ratio $\alpha$ from the Benzeggagh-Kenane relation (2.29) is related to the components of the effective traction:

$$\alpha = \frac{(t_{\text{eff}sh})^2}{(t_{\text{eff}nh})^2 + \langle t_{\text{eff}}^m \rangle^2} \quad (2.43)$$

and that the actual energy dissipation can be expressed as

$$G_T = G_I + G_{II} = \frac{\kappa_f^f F_2^2 \alpha}{2T} \quad (2.44)$$

with

$$F_\alpha^2 = \frac{F_2^2 F_{12}^2}{(1 - \alpha) F_{12}^2 + \alpha F_{2t}^2} \quad (2.45)$$

With these relations, the value of $\kappa_f^f$ in Equation (2.40) is defined as a function of $\alpha$ such that the amount of energy dissipated for different mixed mode cases matches the assumed material behavior. Equalizing $G_{TE}$ in (2.29) to $G_T$ in (2.44) and solving for $\kappa_f^f$ gives:

$$\kappa_f^f = \frac{2T}{F_\alpha^2} (G_{Ic,m} + (G_{IIc,m} - G_{Ic,m}) \alpha^n) \quad (2.46)$$
Because equilibrium was assumed in the derivation of Equation (2.44), while equilibrium is only weakly met, the amount of energy dissipated in the numerical results does not satisfy Equation (2.29) exactly, but it approaches the correct value upon mesh refinement.

Now that the formulation is complete, the significance of the stiffness parameter $T$ is clarified. Figure 2.9 gives a 1D representation of the evolution of different variables with increasing displacement jump, assuming that equilibrium is satisfied exactly. The straight descending line depicts the traction (and at the same time the bulk stress, since those two are in equilibrium). The increasing straight line is the effective traction. The significance of $T$ is that it determines the slope of this line. As a consequence, it influences the ratio between the ‘displacement jump part’ and the ‘bulk stress part’ of the traction (indicated with the dotted curve), and therewith the influence of substituting $\sigma$ for $t$ in Equation (2.35). In the limit for $T \to \infty$, the direct traction separation law from Equation (2.33) is obtained exactly. While, with a finite value for $T$, it is only weakly met. A lower bound for $T$ is given by the requirement that $t_{\text{eff}}$ must be growing during crack opening, i.e. that $\kappa^f > 1$. With Equation (2.46) this requirement becomes:

$$T > \frac{F_n^2}{G_T(\alpha)} \quad \forall \quad \alpha \in [0, 1] \quad (2.47)$$

**Linearization**  For the linearization of the two overlapping elements in the phantom node method, the presence of the bulk stress gives rise to an extra term with respect to Equation (1.29). It now reads

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_A & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_B \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{[u]} & -\mathbf{K}_{[u]} \\ -\mathbf{K}_{[u]} & \mathbf{K}_{[u]} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_\sigma & \mathbf{K}_\sigma \\ -\mathbf{K}_\sigma & -\mathbf{K}_\sigma \end{bmatrix} \quad (2.48)$$
Chapter 2 Constitutive ply modeling

\[ K[u] = T \int_{\Gamma_c} N^T A N \, d\Gamma \]  

\[ K_\sigma = \int_{\Gamma_c} N^T A H DB \, d\Gamma \]  

and

\[ A = \frac{\partial t}{\partial t_{\text{eff}}} = I - \Omega - t \left( \frac{\partial \omega_m}{\partial t_{\text{eff}}} \right)^T \]  

The derivative \( \frac{\partial \omega_m}{\partial t_{\text{eff}}} \) is expanded with the chain rule as

\[ \frac{\partial \omega_m}{\partial t_{\text{eff}}} = \frac{\partial \omega_m}{\partial \kappa} \frac{\partial \kappa}{\partial t_{\text{eff}}} + \frac{\partial \omega_m}{\partial \kappa_f} \frac{\partial \kappa_f}{\partial \alpha} \frac{\partial \alpha}{\partial t_{\text{eff}}} \]  

with

\[ \frac{\partial \omega_m}{\partial \kappa} = \frac{\kappa_f}{\kappa^2(\kappa_f - 1)} \]  

\[ \frac{\partial \kappa}{\partial t_{\text{eff}}} = \frac{1}{\kappa} \left\{ \left( \frac{F_{12}}{F_{22}} \right)^2, \frac{F_{12}}{F_{22}}, \frac{F_{12}}{F_{22}} \right\}^T \]  

\[ \frac{\partial \omega_m}{\partial \kappa_f} = \frac{1 - \kappa}{\kappa(\kappa_f - 1)^2} \]  

\[ \frac{\partial \kappa_f}{\partial \alpha} = \frac{2T}{F_{22}^2} (G_{H_c,m} - G_{E,m}) \eta \alpha^{\eta - 1} - \kappa_f (1 - \alpha) F_{12}^2 + \alpha F_{22}^2 \]  

\[ \frac{\partial \alpha}{\partial t_{\text{eff}}} = 2\alpha (1 - \alpha) \left\{ \frac{1}{\left( t_{\text{eff}}/t_{n} \right)^2}, \frac{t_{\text{eff}}}{t_{n}}, \frac{t_{\text{eff}}}{t_{n}} \right\}^T \]  

Verification The performance of the cohesive law is assessed with mixed mode bending tests. Material parameters from Camanho et al. [13] for carbon/PEEK fiber reinforced composite are used (see Table 2.2). The response is governed by the fracture energy of the material. Therefore, these tests are particularly suitable to verify whether actual dissipation in the simulated response is equal to the input.

The setup for the mixed mode bending test is shown in Figure 2.10. In the experimental setup, the length of the loading arm, \( c \), governs the mode ratio. In the computational model, however, the ratio between the two point loads \( F_m \) and \( F_e \) is fixed instead of modeling the loading arm. The mode I test (double cantilever beam) is obtained by setting \( F_m \) equal to zero, and the mode II test (end notched flexure) is obtained by replacing \( F_e \) with a nodal displacement constraint. Theoretical solutions exist for all mixed mode bending tests, derived from theoretical solutions for
2.3 Bulk stress constrained cohesive law

\[ F, u \]

\[ L = 100 \text{ mm} \]

\[ h = 3.12 \text{ mm} \]

\[ c, a \]


---

**Figure 2.10** Mixed mode bending test setup (left) and computational model (right).

**Table 2.2** Material parameters for mixed mode bending tests, taken from [13].

<table>
<thead>
<tr>
<th>Elasticity</th>
<th>Matrix cracking</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_1 ) 122.7 GPa</td>
<td>( P_{21} ), 80 MPa</td>
</tr>
<tr>
<td>( E_2 ) 10.1 GPa</td>
<td>( F_{12} ), 100 MPa</td>
</tr>
<tr>
<td>( \nu_{21} ) 0.25</td>
<td>( G_{I_{e,m}} ), 0.969 N/mm</td>
</tr>
<tr>
<td>( G_{12} ) 5.5 GPa</td>
<td>( G_{II_{e,m}} ), 1.719 N/mm</td>
</tr>
</tbody>
</table>

...the extreme cases. With beam theory and the assumption that the fracture energy is constant, the force and displacement during crack propagation for each value of crack length \( a \) can be obtained.

**Figure 2.11** shows the relations between load and displacement obtained with the presented model for the two pure mode and three mixed mode cases. Theoretical curves are also shown. For this, relations are used that were concatenated by Reeder and Crews [105] from the work of Kanninen [51], Whitney et al. [133] and Carlsson et al. [17]. For the mixed mode cases, the eccentric load \( F \) is plotted against the deflection of the loading point \( u \), while for the pure mode cases it is \( F_e \) against

![Figure 2.11](image-url)

**Figure 2.11** Verification of constrained cohesive law: load-displacement relation for mixed mode bending with five different values of the mode ratio, compared with theory.
$u_e$ and $F_m$ against $u_m$. It can be observed that agreement is excellent, at least as far as the initial stiffness and the descending branch are concerned. The agreement in peak load value is not that well. This can be explained by the fact that in the theoretical solution, there is no cohesive zone. In the numerical model, the cohesive zone is already developing in the ascending branch. The peak load corresponds with the moment at which complete local failure is reached for the first time, i.e. when the cohesive zone has fully developed. At that point, there has already been some loss in stiffness, which can be interpreted as an increase of the effective crack length.

It is concluded that the cohesive law indeed gives the correct results. In a more detailed study, it has been found that the results are insensitive to the value of $T$ as long as it is chosen at least equal to $10^5$ N/mm$^3$ and, furthermore, that convergence is optimal for $T \in [10^5, 10^6]$ N/mm$^3$.

### 2.4 Shifted cohesive law

Another way to construct an initially rigid law without singularity has been proposed by Hille et al. [43]. Here, the idea is to start from a traction separation relation with a finite initial stiffness and to shift this relation such that the traction for zero crack opening is equal to the traction at crack initiation. This technique can be applied to any traction-separation law with high initial stiffness by simply applying a translation to the input of the constitutive law. In this section, it is applied to the mixed mode damage law developed for interface elements by Turon et al. [122].

**Traction update** Starting point is the damage law in its original form, which is denoted: $T_\omega$. The law relates the evolution of the traction $t$ to the evolution of displacement jump $[u]$ as

$$ t(t) = T_\omega ([u](t)) $$

where the argument $(t)$ is used to indicate the history dependency of $T_\omega$. This law is modified by applying a translation to the input argument. The traction is computed not from the actual displacement jump $[u]$, but from a translated displacement jump $[v]$:

$$ t(t) = T_\omega ([v](t)) $$

with

$$ [v](t) = [u](t) + [u]^0 $$

The shift $[u]^0$ is computed from the bulk stress at the moment of crack initiation, such that the shifted damage law gives $t = \sigma n$ for zero damage and zero opening.
2.4 Shifted cohesive law

For zero damage, the Turon damage law is linear elastic:

\[ t = K_m \llbracket u \rrbracket \]  

(2.61)

In other words, the shift \( \llbracket u \rrbracket^0 \) should satisfy \( K_m \llbracket u \rrbracket^0 = \sigma n \). Therefore, it is defined as

\[ \llbracket u \rrbracket^0 = \frac{1}{K_m} \sigma n \]  

(2.62)

This leads to the desired initially rigid behavior (see Figure 2.12). Moreover, the traction-separation relation is uniquely defined everywhere as long as \( K_m \) is finite. When the loading is non-monotonic, it is possible that the sign of the traction is not equal to that of the displacement jump. Moreover, due to the shift the actual energy dissipation is not exactly equal to input value. But the effect of both of these flaws is limited as long as \( K_m \) is chosen sufficiently high. In the limit for \( K_m \to \infty \), the shift vanishes, and the ideal initially rigid law is regained, together with the singular behavior.

The effective traction is defined as

\[ t_{\text{eff}} = K_m \llbracket v \rrbracket \]  

(2.63)

Then the traction update in the local \( \{ n, s, t \} \)-frame with prevention of interpenetration is exactly equal to that for the bulk stress constrained cohesive law:

\[ t = [I - \Omega] t_{\text{eff}} \]  

(2.36)

\[ \Omega_{ij} = \omega_m \delta_{ij} \left( 1 - \delta_{i1} \frac{t_{n_{\text{eff}}}}{t_{n_{\text{eff}}}} \right) \]  

(2.37)

Figure 2.12 Pure mode I representation of shift in cohesive law to mimic initially rigid behavior.
Damage evolution  Following Turon et al. [122], the monotonically increasing damage variable $\omega_m$ is defined as

$$
\omega_m = \max_{\tau \leq t} \left\{ \begin{array}{ll}
0, & \mathcal{U}_\text{eq} \leq \mathcal{U}_\text{eq}^0 \\
\mathcal{U}_\text{eq} \left( \mathcal{U}_\text{eq} - \mathcal{U}_\text{eq}^0 \right), & \mathcal{U}_\text{eq}^0 < \mathcal{U}_\text{eq} < \mathcal{U}_\text{eq}^f \\
1, & \mathcal{U}_\text{eq} \geq \mathcal{U}_\text{eq}^f
\end{array} \right. 
$$

(2.64)

But, in this case, the equivalent displacement jump is the norm of the shifted displacement jump vector

$$
\mathcal{U}_\text{eq} = \sqrt{\langle \mathcal{V}_n \rangle^2 + \langle \mathcal{V}_\text{sh} \rangle^2}
$$

(2.65)

with

$$
\langle \mathcal{V}_\text{sh} \rangle^2 = \langle \mathcal{V}_n \rangle^2 + \langle \mathcal{V}_\text{sh} \rangle^2
$$

(2.66)

The values for the equivalent displacement jump that mark onset of failure and complete damage match the Benzeggagh-Kenane relation Equation (2.29):

$$
\mathcal{U}_\text{eq}^0 = \sqrt{\langle \mathcal{V}_n \rangle^2 + \left( \langle \mathcal{V}_\text{sh} \rangle^2 - \langle \mathcal{V}_n \rangle^2 \right)^2} \alpha^n
$$

(2.67)

$$
\mathcal{U}_\text{eq}^f = \frac{\mathcal{U}_\text{eq}^0 \langle \mathcal{V}_n \rangle^f + \left( \mathcal{U}_\text{eq}^0 \langle \mathcal{V}_\text{sh} \rangle^f - \langle \mathcal{V}_n \rangle^f \mathcal{U}_\text{eq}^f \right)}{\mathcal{U}_\text{eq}^0} \alpha^n
$$

(2.68)

with

$$
\mathcal{U}_n^0 = \frac{F_{2t}}{K_m}, \quad \mathcal{U}_n^f = \frac{2G_{Ic,m}}{F_{2t}}
$$

(2.69)

$$
\mathcal{U}_\text{sh}^0 = \frac{F_{12}}{K_m}, \quad \mathcal{U}_\text{sh}^f = \frac{2G_{IIc,m}}{F_{12}}
$$

(2.70)

In the constitutive law, the ratio $\alpha$ is computed from the displacement jump components as

$$
\alpha = \frac{\beta^2}{1 + 2\beta^2 - 2\beta}
$$

(2.71)

$$
\beta = \frac{\langle \mathcal{V}_\text{sh} \rangle}{\langle \mathcal{V}_n \rangle + \langle \mathcal{V}_\text{sh} \rangle}
$$

(2.72)

Failure criterion  With the bulk stress constrained cohesive law, it was necessary for continuity of the response to use a failure criterion that matched the damage evolution. With the shifted cohesive law, however, continuity of the failure criterion
is naturally ensured as long as the initial traction $\sigma_n$ can be located on the original traction-separation relation. For the presented formulation, the shift is such that the initial traction coincides with the maximum of the traction separation law when new crack segments are introduced for

$$\frac{(\sigma_2)^2 + \tau_{sh}^2}{F_{2a}^2 + (F_{2a}^2 - F_{2a}^2) \alpha^2} = 1$$

(2.73)

where $\alpha$ is defined with Equation (2.71) and

$$\beta = \frac{\tau_{sh}}{\tau_{sh} + (\sigma_2)}$$

(2.74)

In principle, however, crack segments can be introduced before the maximum traction in the cohesive law has been reached. In that case the shift is smaller than indicated in Figure 2.12, which results in a traction-separation law that starts with a positive gradient. One could expect this to be beneficial for the convergence, since two possible sources of instability, the introduction of crack segments and the onset of softening, are thus disconnected. In our experience, in some cases divergence could be avoided with such early insertion of crack segments, but in general, convergence was slower. Occasional divergence is surmountable with adaptive stepping (see Chapter 4), and for the examples shown in this thesis, the extra computational costs due to general slow convergence are larger than those due to occasional non-convergence. Therefore, the value of one on the right hand side of Equation (2.73) is maintained.

**Linearization** In contrast with the constrained cohesive law presented in the previous section, the shifted cohesive law computes the traction directly from the displacement jump. Therefore its linearization is as presented in Equation (1.29). The gradient of traction with respect to displacement jump, which enters the formulation in matrix $T$, is not affected by the shift itself and is therefore equal to the standard linearization of the Turon constitutive law. This gradient which will be defined when the original law without shift is presented for modeling of delamination in Section 3.1.

**Verification** Like in the previous section, the cohesive law is tested with the simulation of a series of mixed mode bending tests. In Figure 2.13 the load-displacement relations are plotted in comparison with theoretical curves. The same parameters are used, with a single addition, namely the dummy stiffness, which is $K_m = 10^6$ N/mm$^3$. Again, an excellent match with the theoretical response is obtained.

Varying the dummy stiffness $K_m$ has shown that a decrease led to better convergence behavior. Obviously, decreasing $K_m$ too much leads to inaccuracy, because
the shift grows and the actual energy dissipation is reduced. For $K_{m} = 10^6$ and the parameters in Table 2.2, the error in the effective fracture energy for a fixed mode case is at most 0.5%.

2.5 Fiber failure

In order to build a complete model for ply failure, the discontinuous model for matrix cracking is combined with a continuum damage model for fiber failure, see Figure 2.15(a). Several considerations have led to the preference of a continuum damage model over a discontinuous approach here. Firstly, the compelling reason to use a discontinuous representation for matrix cracks, namely that the direction of crack propagation is governed by the microstructure rather than by the stress field, is not present in this case. Moreover, in the case in which a band with fiber failure grows in the direction of a matrix crack in an adjacent ply, the discontinuous approach will have more difficulty in predicting this orientation. Prior to failure there is a band of elements in which stress is high. With a continuum model this will automatically lead to failure in this band, while it is not clear how this propagation direction should be extracted from the stress field in case it is modeled as a propagating discontinuity in the displacement field. Secondly, the continuum description fits the physics well, because fiber failure is a mechanism that results in a band in which material is damaged. This is due to the fact that fibers do not fail in a smooth plane, the process generally involves pull out of fibers from a zone with extensive matrix failure.

The remaining disadvantage of the continuum approach to failure is that regularization is needed. Here, the crack band method [4] is employed. This simple method, in which the constitutive behavior depends on the element size, leads to mesh size independent results, although limited dependence on the orientation of the mesh may still be present. More advanced nonlocal damage theories such as the implicit
2.5 Fiber failure

Gradient damage model by Peerlings et al. [96] are theoretically more sound, but require a very fine mesh in the damaged zone.

**Stress update**  Because the fiber failure mechanism does not leave the matrix intact, isotropic softening is assumed

$$\sigma = (1 - \omega_f) D^e \varepsilon$$  \hspace{1cm} (2.75)

The force that drives degradation, however, is orthotropic, motivated by the obvious fact that fiber failure only occurs due to loading in fiber direction. Puck and Schürmann [102] argued that the difference between available formulations is small as far as failure initiation is concerned. Therefore, for simplicity, maximum strain and maximum stress criteria are to be preferred. Of these, the maximum strain criterion is most appropriate to drive the degradation, because this largely rules out the influence of transverse strain on the amount of energy dissipated due to fiber failure. The variable $\kappa_f$ is defined as the time maximum of the normalized strain in fiber direction

$$\kappa_f = \frac{E_1 \langle \varepsilon_1 \rangle}{F_{1t}}$$  \hspace{1cm} (2.76)

where $E_1$ is the ply Young’s modulus in fiber direction, $\langle \varepsilon_1 \rangle$ is the positive strain in fiber direction and $F_{1t}$ is the ply strength in fiber direction. Damage initiates when $\kappa_f = 1$ and an exponential softening relation is used to compute $\omega_f$.

$$\omega_f = \max_{\tau \leq t} \begin{cases} 0, & \kappa_f \leq 1 \\ 1 - \frac{1}{\kappa_f} e^{-\beta(\kappa_f - 1)}, & \kappa_f > 1 \end{cases}$$  \hspace{1cm} (2.77)

where $\beta$ is related to the fracture energy.

For a most realistic representation of crack bridging behavior as observed by Pinho et al. [99], linear-exponential [70] or bilinear [22] softening would be better, but for the current investigations the formulation is kept as simple as possible.

**Regularization**  The crack band method is applied for regularization [4], i.e. a characteristic element length is discounted in the local constitutive behavior. The energy that should be dissipated for fracture energy $G_{k,t}$ in a band with volume $V$ and width $L^*$ is:

$$E_{\text{theory}} = G_{k,t} \frac{V}{L^*}$$  \hspace{1cm} (2.78)

The actual energy that is dissipated when this band is completely damaged (assuming $\beta$ does not vary within the volume) is

$$E_{\text{actual}} = \int_V \int_0^\infty (1 - \omega_f) E_1 \varepsilon_1 \, d\varepsilon \, dV = V \frac{F_{1t}^2}{E_1} \left( \frac{1}{2} + \frac{1}{\beta} \right)$$  \hspace{1cm} (2.79)
The relation between $\beta$ and $L^*$ can be obtained by equating $E_{\text{theory}}$ with $E_{\text{actual}}$. This results in:

$$\beta = \frac{2L^* F_1^2}{2G_{h,1}E_1 - L^* F_1^2}$$

(2.80)

Obviously, since failure localizes in a single layer of elements, the width of the fracture band is related to the element size. The crack band width is assumed to be equal to the averaged projected length $b$ of an arbitrarily oriented equilateral triangle with side length $a$ (see Figure 2.14):

$$L^* = \frac{6}{\pi} \int_0^{\frac{\pi}{6}} b d\phi = \frac{3}{\pi} a$$

(2.81)

With the relation between $a$ and the area $A$

$$A = \frac{\sqrt{3}}{4} a^2$$

(2.82)

this relation becomes

$$L^* = \frac{6}{\pi} \sqrt{\frac{A}{\sqrt{3}}}$$

(2.83)

This estimate is not optimal for the crack band width indicated with $L'$ in Figure 2.14. There remains a mesh dependency in the sense that the mesh alignment with respect to the crack path influences the actual energy dissipation.

**Interaction with matrix cracks** For the influence of fiber failure on the matrix cracking process the assumption of isotropic softening is maintained. That means, firstly, that the failure criterion is applied on the effective stress ($D^* \varepsilon$) instead of on the nominal stress $\sigma$ and, secondly, that after crack initiation fiber damage is also applied to the traction

$$t = (1 - \omega_f)(1 - \omega_m) t_{\text{eff}}$$

(2.84)
where \((1 - \omega_m) t^{\text{eff}}\) is traction as computed with the cohesive law (see Section 2.3 or 2.4). In each cohesive integration point, \(\omega_f\) is computed from the bulk strain at that point, which is taken as the average of the independent strains on both sides of the crack.

### 2.6 Shear nonlinearity

A final feature is added to the constitutive model of the ply. This is related to nonlinear deformations in the matrix, which can be substantial before failure, particularly in shear. Van Paepegem et al. [125, 126] have proposed a phenomenological model for shear nonlinearity which includes both damage and plasticity, so that it can be fitted with respect to observed loading/unloading behavior with both stiffness degradation and permanent strain, see Figure 2.15(b). For failure analysis, a proper description of the unloading behavior is of importance, also under monotonic boundary conditions, because unloading of the bulk material will occur around the failure zone.

**Stress update**  The basic relation between shear stress and shear strain with damage and plasticity is

\[
\tau_{12} = G_{12} (1 - \omega_{12}) (\gamma_{12} - \gamma_{12}^P)
\]  

(2.85)

Van Paepegem et al. [125] give exponential evolution relations for \(\omega_{12}\) and \(\gamma_{12}^P\) in differential form. In order to obtain behavior that is independent of the time step
size, the equations are rewritten here in closed form:

\[
\frac{d\gamma_{12}^p}{d\gamma_{12}} = C_1 \gamma_{12} \exp (C_2 \gamma_{12}^p) \Rightarrow \gamma_{12}^p = -\frac{\ln (1 - C_1 C_2 \gamma_{12}^p/2)}{C_2} \tag{2.86}
\]

\[
\frac{d\omega_{12}}{d\gamma_{12}} = C_3 \exp (C_4 \omega_{12}) \Rightarrow \omega_{12} = -\frac{\ln (1 - C_3 C_4 \gamma_{12})}{C_4} \tag{2.87}
\]

Apart from the elimination of the differential formulation, another change has been made in Equation (2.87) with respect to the original formulation. Namely that the evolution of \( D \) depends on the total strain \( \gamma_{12} \) rather than on the elastic strain \( \gamma_{12}^e = \gamma_{12} - \gamma_{12}^p \). This adaptation disentangles the influence of the four material parameters \( C_1 \ldots C_4 \) on the stress strain behavior and therefore simplifies the curve fitting exercise in which these parameters are to be obtained.

In laminate analysis, matrix cracking will not be allowed everywhere in the domain (see Section 3.3). As a consequence, it cannot be excluded that the stress in the bulk material between two cracks will exceed the matrix strength. For this reason, the model for shear nonlinearity, needs to remain well-posed beyond the failure strain, even though it is unclear what is the physical meaning of this part. The model by Van Paepegem et al. [125] starts to exhibit softening from a certain threshold strain. This would violate the separation between matrix nonlinearity and matrix failure and is therefore undesirable. This is solved by extending the phenomenological curve with a perfectly plastic part beyond the point where \( \partial \gamma_{12}/\partial \gamma_{12} = 0 \).

**Interaction with other processes** The interaction between shear nonlinearity and fiber damage is straightforward because the two processes are driven by independent strain components. Fiber damage is applied to the total stress after shear nonlinearity, i.e. Equation (2.75) is generalized to

\[
\sigma = (1 - \omega_f) \hat{D} \varepsilon^e \tag{2.88}
\]

where \( \hat{D} \) is the orthotropic material stiffness matrix with nonlinear shear component \( \hat{D}_{66} = (1 - \omega_{12}) G_{12} \) and \( \varepsilon^e \) is the elastic strain with \( \gamma_{12}^e = \gamma_{12} - \gamma_{12}^p \).

There is no coupling between hardening matrix damage \( \omega_{12} \) and softening matrix damage in transverse cracks (\( \omega_m \)) or in the interface (\( \omega_i \)). This can only be justified if the microcracks that are represented by \( \omega_{12} \) in the continuum are not aligned with the microcracks represented by \( \omega_m \) and \( \omega_i \) in the cohesive zones. For delamination this is a likely assumption, but for transverse cracking some kind of interaction would be realistic. Moreover, where parameter identification is concerned, in the measurement of \( G_{IIc,m} \) there is definitely some energy dissipation involved that is due to the very same processes that are interpreted as shear nonlinearity in other measurements. The sharp distinction between matrix damage in transverse cracks
2.6 Shear nonlinearity

and matrix damage due to in plane shear is debatable. This is a consequence of the mesolevel approach. Two phenomena are dealt with that are clearly distinct on the mesoscale but nevertheless connected on the microscale. For now, this issue is left unresolved, because energy dissipation in matrix cracks is not the most important property in the complete failure simulation.

In combination with the continuum damage model for fiber failure and the phantom node method with one of the two cohesive laws for matrix cracking, the numerical model for ply failure is complete. This model allows for realistic simulation of the different processes during failure of a unidirectional composite material in tensile load cases. But meaningful validation of the model is not possible on the level of the single ply. Complex failure mechanisms with interaction between the different processes are only manifest in full laminate analysis, i.e. when several unidirectional plies are stacked together.
Chapter 3 Laminate analysis

In the previous chapter, a constitutive model for the elementary ply has been introduced. Now, this will be extended towards a framework for complete laminate analysis. The numerical model for the laminate consists of one layer of elements per ply and interface elements between the plies. The elements for the ply are either three-dimensional solid or plane stress elements. In the latter case, the through-thickness layup of the laminate is mimicked, by connecting neighboring plies with interface elements, even though no z-coordinates are present. Delamination can then also be captured in plane stress, although, in absence of out-of-plane degrees of freedom, only sliding relative displacements are captured.

For the analysis of laminate failure, one more constitutive model is needed, namely for failure between the plies or delamination. After the interface elements for delamination are added, the discontinuous approach to matrix cracks introduced in the previous chapter again demands attention. In a complete laminate, matrix cracks in a single ply do not lead to failure because of mutual constraint of the plies. A matrix crack in one ply is closed by the fibers in neighboring plies. This is the cause for the phenomenon of distributed cracking: arrays of matrix cracks may appear before the laminate breaks. When a matrix crack is closed by the neighboring plies, stress is transferred via the ply interface, which may trigger delamination.

In Section 3.1 the constitutive model for the interface is presented. Next, in Section 3.2, the interaction of the interface elements for delamination with the phantom node method for matrix cracking is investigated. In Section 3.3, distributed cracking is considered and a crack spacing parameter for matrix cracking is introduced to keep the problem well-posed. Finally, in Section 3.4 it is shown that neglecting out-of-plane deformations can be acceptable in full laminate analysis with delamination and matrix cracking.

Several numerical examples are shown with which the reliability of the framework is verified. In-depth validation including a comparison with experimental observations will be endeavored in Chapter 5.

3.1 Constitutive model for delamination

The mixed-mode damage law developed by Turon et al. [122] is used in the interface elements. This cohesive law incorporates the phenomenological relation between
fracture toughness and mode ratio proposed by Benzeggagh and Kenane [9]. In plane stress analyses, the same law is used, albeit trivialized by the plane stress postulate \( \| u \|_n = 0 \). It reduces to a simple bilinear law (see Figure 3.1). Furthermore, in plane stress, a finite value with physical meaning can be assigned to the dummy stiffness \( K_d \) which ought otherwise be chosen as high as numerical stability allows. Now, elastic deformation of the interface can be related to out-of-plane shear deformation.

**Traction update** The traction and displacement jump are defined in the local frame that is aligned with crack surface, with the first component normal to that surface. The traction is computed from the displacement jump with isotropic damage and prevention of interpenetration as:

\[
t = (I - \omega_d P)K_d \langle u \rangle
\]  

(3.1)

with

\[
P = \begin{bmatrix}
\langle \frac{\| u \|}{\| \dot{u} \|} \rangle & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\]  

(3.2)

where \( \omega_d \) is the damage variable, and the matrix \( P \) is included to cancel the influence of damage in the normal direction in case of compression, using the operator \( \langle x \rangle = (x + |x|)/2 \). The damage variable is defined as

\[
\omega_d = \max_{\tau \leq t} \begin{cases}
0, & \| u \|_{eq} \leq \| u \|_{eq}^0 \\
\| u \|_{eq}^f / \| u \|_{eq}^f - \| u \|_{eq}^0, & \| u \|_{eq}^0 < \| u \|_{eq} < \| u \|_{eq}^f \\
1, & \| u \|_{eq} \geq \| u \|_{eq}^f
\end{cases}
\]  

(3.3)
3.1 Constitutive model for delamination

with

\[ [u]_{eq} = \sqrt{([u]_n)^2 + [u]_{sh}^2} \] (3.4)

\[ [u]_{eq}^0 = \sqrt{([u]_n^0)^2 + \left(([u]_{sh}^0)^2 - ([u]_n^0)^2\right)} \alpha \eta \] (3.5)

\[ [u]_{eq} = \frac{[u]_{sh}^0 [u]_{n}^0 + (1 - [u]_{sh}^0 [u]_{sh}^0 - [u]_{n}^0 [u]_n^0) \alpha \eta}{[u]_{eq}^0} \] (3.6)

\[ \alpha = \frac{G_{II}}{G_I + G_{II}} = \frac{[u]_{sh}^2}{[u]_{sh}^2 + ([u]_n^0)^2} \] (3.7)

and

\[ [u]_{sh}^2 = ([u]_n^2 + [u]_{sh}^2) \] (3.8)

\[ [u]_n^0 = \frac{F_{3t}}{K_d}, \quad [u]_{sh}^0 = \frac{2G_{Ic,d}}{F_{3t}} \] (3.9)

\[ [u]_{sh}^0 = \frac{F_{sh}}{K_d}, \quad [u]_{sh}^0 = \frac{2G_{IIc,d}}{F_{sh}} \] (3.10)

where \( F_{3t} \) and \( F_{sh} \) are the tensile and shear strength, \( G_{Ic,d} \) and \( G_{IIc,d} \) are the mode I and mode II fracture toughness and \( \eta \) is the Benzeggagh-Kenane interaction parameter [9]. Throughout this work, the strength and toughness properties for delamination are equated to those for matrix cracking, i.e. \( F_{3t} = F_{2t}, F_{sh} = F_{12}, G_{Ic,d} = G_{Ic,m} \) and \( G_{IIc,d} = G_{IIc,m} \). On first sight this is reasonable, because from micromechanical point of view delamination is also cracking of the matrix material. On closer inspection, however, the fact that delamination occurs in the resin rich area between the plies is likely to influence the properties. The process of cusp formation, for instance, which contributes to the energy dissipation in mode II delamination (see Greenhalgh et al. [30]), can only take place in the resin region between the plies. Moreover, there is evidence that the delamination properties depend on the relative orientation of the neighboring plies [30]. But the availability of independently measured values is limited and therefore the examples in this thesis are based on a single set of parameters \( F_{3t}, F_{12}, G_{Ic,m}, G_{IIc,m} \) and \( \eta \) for both transverse and interply matrix failure.

Notably, the damage law deviates from the original formulation by Turon et al. [122] at one point, namely that \( \omega_d \) is used as state variable instead of \( [u]_{eq} \) (the max-operator appears in Equation (3.3) rather than in Equation (3.6)). For pure mode cases, both are equivalent, but for varying mode ratio there can be a small influence. Using \( \omega_d \) for this purpose is more consistent with the interpretation of damage as the growth of voids and microcracks. Because in this interpretation, the damage variable is the ratio between the cracked and the intact part of the surface, and as such a measure for the state of the material, whereas the equivalent displacement jump is a measure for the deformation. The first is irreversible, the second is not.
Linearization  During damage growth, the consistent tangent for this constitutive model is defined as

\[ D = K_d \left[ I - \omega_d P - P [u] \left( \frac{\partial \omega_d}{\partial [u]} \right)^T \right] \]  

(3.11)

with (see Equation (3.3)):

\[ \frac{\partial \omega_d}{\partial [u]} = \frac{\partial \omega_d}{\partial [u]_{eq}} \frac{\partial [u]_{eq}}{\partial [u]} + \frac{\partial \omega_d}{\partial [u]_{eq}} \frac{\partial [u]_{eq}^0}{\partial [u]} + \frac{\partial \omega_d}{\partial [u]_{eq}} \frac{\partial [u]_{eq}^f}{\partial [u]} \]  

(3.12)

Notably, in the paper by Turon et al. [122] the last two terms of (3.12) are left out of consideration. Although these terms generally are small, in analyses with multiple interacting nonlinear processes such as considered here, fully consistent linearization is crucial and these terms must be included to obtain convergence. Equation (3.12) is expanded with

\[ \frac{\partial \omega_d}{\partial [u]_{eq}} = \frac{\partial f}{\partial [u]_{eq}} \left( \frac{[u]_{eq}^f}{[u]_{eq}} - \frac{[u]_{eq}^0}{[u]_{eq}} \right) \]  

(3.13)

\[ \frac{\partial [u]_{eq}}{\partial [u]} = \frac{1}{[u]_{eq}^1} [u] \]  

(3.14)

\[ \frac{\partial [u]_{eq}^0}{\partial [u]_{eq}} = \frac{\partial [u]_{eq}^0}{\partial [u]_{eq}} \frac{\partial \alpha}{\partial \alpha} \frac{\partial \alpha}{\partial [u]} \]  

(3.15)

\[ \frac{\partial [u]_{eq}^0}{\partial [u]} = \frac{\partial [u]_{eq}^0}{\partial [u]_{eq}} \frac{\partial \alpha}{\partial \alpha} \frac{\partial \alpha}{\partial [u]} \]  

(3.16)

\[ \frac{\partial [u]_{eq}^f}{\partial [u]_{eq}} = \frac{\partial [u]_{eq}^f}{\partial [u]_{eq}} \frac{\partial \alpha}{\partial \alpha} \frac{\partial \alpha}{\partial [u]} \]  

(3.17)

\[ \frac{\partial [u]_{eq}^0}{\partial [u]} = \frac{\partial [u]_{eq}^0}{\partial [u]_{eq}} \frac{\partial \alpha}{\partial \alpha} \frac{\partial \alpha}{\partial [u]} \]  

(3.18)

and

\[ \frac{\partial [u]_{eq}^0}{\partial \alpha} = \left( [u]_{eq}^0 \right)^2 - \left( [u]_{eq}^0 \right)^2 \]  

(3.19)

\[ \frac{\partial [u]_{eq}^f}{\partial \alpha} = \frac{[u]_{eq}^f}{[u]_{eq}^0} \frac{\partial [u]_{eq}^0}{\partial [u]_{eq}} + \frac{[u]_{eq}^0 [u]_{eq}^f [u]_{eq}^f}{[u]_{eq}^0} \]  

(3.20)

\[ \frac{\partial \alpha}{\partial \alpha} = \eta \alpha^{\eta - 1} \]  

(3.21)

\[ \frac{\partial \alpha}{\partial [u]} = 2\alpha (1 - \alpha) \left\{ -\frac{1}{[u]_{eq}^0}, \frac{[u]_{eq}^0}{[u]_{eq}^2}, \frac{[u]_{eq}^0}{[u]_{eq}^2} \right\}^T \]  

(3.22)
3.2 Interaction between matrix cracks and delamination

This section deals with the numerical representation of the interaction between matrix cracks and delamination when the former is modeled with the phantom node method and the latter with interface elements. The investigations are performed in a two-dimensional framework where each ply is modeled with a single layer of plane stress elements, but the same holds for a three-dimensional framework with one layer of solid elements per ply.

When a discontinuity appears in the displacement field of one of the planes that are connected with interface elements, this obviously affects the relative displacement field between the planes. Application of the phantom node method for the ply theoretically requires that the interface elements connecting the plies are adapted, as shown in Figure 3.2. Each of the plane displacement fields $\mathbf{N}_\text{bottom}$ and $\mathbf{N}_\text{top}$ in the definition of the interface displacement jump in Equation (1.17) may become discontinuous as in Equation (1.25). This should be taken into account in the evaluation of the interface displacement jump. Practically, this would entail that upon introduction of phantom nodes, the connectivity and integration scheme of the interface elements is adapted accordingly, including transfer of history variables. Moreover, the possibility that both connected planes in a single interface element are cracked has to be accounted for.

However, with the phantom node method, more than with traditional partition of unity based methods, the nodal displacements related to the original nodes of a cracked element remain meaningful, due to the fact that those are always in the active part of the overlapping elements (see Figure 1.6). When the interface elements are not adapted upon cracking of the plies, the inconsistency in the displacement field is limited to the interior of the element. Since high accuracy in the displacement field at sub-element level is generally not pursued in finite element analysis, the consequences of using such a nonconforming displacement field may very well be acceptable. Moreover, the significance of an error at sub element level will vanish.
Transverse crack initiation
Minor delamination
Major delamination

Solid elements for plies
Decohesion of phantom node crack

Interface integration pt.
Load transfer via interface
Delamination damage

**Figure 3.3** Interaction between matrix cracking and delamination: sketch of real deformations (top) and numerical representation with unadapted interface element and nodal integration (bottom).

Upon mesh refinement.

At the nodes, the unadapted displacement field is equal to the discontinuous field. The relative displacement between each pair of original nodes remains the real relative displacement of the corresponding pair of material points. Therefore, if a nodal integration scheme is used for the interface element, the displacement jump of the unadapted interface element evaluated at the integration points is exact. Then, not-updating the interface element means not much more than under-integration of the displacement jump field.

Besides that, the use of nodal (Newton-Cotes) integration in interface elements has proved useful to suppress spurious oscillations that may appear in the traction profile when a high dummy stiffness is used (see Schellekens and De Borst [109]). In plane stress analysis, this argument is nullified because then a finite elastic stiffness is appropriate, but it is noteworthy that the use of a nodal integration scheme for interface elements already is a well established practice.

A schematic representation of the mechanical process in which matrix cracking and delamination interact is given in the top row of Figure 3.3. The material in two plies with in-plane dimensions corresponding with a single quadrilateral finite element is considered. First, a matrix crack appears in the transverse ply. Next, significant crack opening demands that minor delamination takes place. Finally, the delamination front propagates beyond the boundaries of the element domain. The numerical representation of the interaction with an unadapted interface element and nodal integration is shown in the bottom row of Figure 3.3. Integration points in the interface element are indicated as springs. With this simplified description, limited crack opening may occur without any delamination. But major delamination will still result in interface damage.

With unadapted interface elements minor delamination is not captured. However, even if they would be adapted, the complex micromechanical stress and displacement
field that corresponds with this state would not be represented accurately. Furthermore, with unadapted elements, the final amount of energy dissipated will be correct when major delamination occurs on both sides of the splitting crack, and will approach the correct value upon mesh-refinement when major delamination occurs on only one side of the crack.

Therefore, unadapted interface elements are used in the proposed laminate model. In the following example, this choice will be validated.

**Open hole laminate** Above, it has been argued that an error is introduced by not updating interface elements when neighboring solid elements are cracked, but that this error can be expected to vanish upon mesh refinement. Here, the magnitude of this error is investigated with a mesh-refinement study for a case in which interaction between splitting and delamination is essential. A \([\pm 45]_s\)-laminate with a circular hole is considered (see Figure 3.4). The nodes on the right and left boundary are constrained in \(x\) and \(y\) direction, with nonzero displacement in \(x\)-direction for the right boundary. The location of two cracks per ply is predefined in order to keep the response relatively simple.

![Figure 3.4 Geometry of cross-ply open hole laminate.](image)

This setup is selected to test the interaction between matrix cracking and delamination, because complete failure of the specimen is possible with those two processes. Matrix cracks are growing from the hole to the long edge. But these cracks alone are not sufficient to form a mechanism, because of mutual constraint between the two plies. The load is transferred via the interface, which causes delamination to grow away from those cracks, until the area between the cracks is completely delaminated. The failure mechanism is illustrated in Figure 3.5 where the deformation short before final failure is shown. It can be observed that failure is complete on one side of the hole, while delamination between the matrix cracks on the other side of the hole is still developing. The asymmetry in the response is due to the unstable nature of the delamination process and it is triggered by asymmetry in the mesh.

The material parameters are summarized in Table 3.1. As proposed in Section 3.1,
Table 3.1 Material parameters for numerical examples in Chapter 3.

<table>
<thead>
<tr>
<th>Elasticity</th>
<th>Failure</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$</td>
<td>$F_{2t}$</td>
</tr>
<tr>
<td>$E_2$</td>
<td>$F_{12}$</td>
</tr>
<tr>
<td>$\nu_{23}$</td>
<td>$G_{IIc,m}$</td>
</tr>
<tr>
<td>$G_{12}$</td>
<td>$G_{Ic,m}$</td>
</tr>
<tr>
<td>$\eta$</td>
<td></td>
</tr>
</tbody>
</table>

Figure 3.5 Deformed mesh from open hole analysis just before final failure; deformations are magnified with a factor 20; the ply thickness is added in postprocessing.

the same strength and fracture energy parameters are used for transverse matrix cracking and delamination. These parameters are used for all numerical examples in this chapter, as well as the ply thickness of 0.5 mm and the elastic interface stiffness of $K_d = G_{12}/(\frac{1}{2}t) = 22 \cdot 10^3$ N/mm$^3$. The bulk stress constrained cohesive law is used with $T = 10^6$ N/mm$^3$.

Six different meshes are used and two different integration schemes for the interface elements. All meshes are generated with the same mesh generator, where the typical element length is each time scaled throughout the domain with a factor $1/\sqrt{2}$, resulting in an increase in the number of nodes with a factor of approximately two. The triangular interface elements are integrated with either a three point Gauss scheme or a three point Newton-Cotes scheme. Load-displacement diagrams for three different meshes are presented in Figure 3.6. The dissipation-based arclength method (see Section 4.1) allows for flawless tracking of the equilibrium path with two sharp snapbacks, each corresponding with delamination on one side of the hole. It can be observed that differences between the results for the different meshes are limited. Especially with the two finer meshes, there is very good agreement between the results.

Figure 3.7 shows the trend in maximum load value upon mesh refinement for both integration schemes. The results are practically equal for all meshes with Newton-Cotes integration. The trend for the peak load value with Gauss integration ap-
3.2 Interaction between matrix cracks and delamination

Figure 3.6 Load-displacement relation for open hole laminate with limited number of cracks obtained with three different meshes and two different integration schemes.

Figure 3.7 Peak load for different meshes for open hole laminate with limited number of cracks.

The total energy dissipation can be computed via integration of the local energy dissipation over the crack surfaces. This results in a scalar quantity that indicates the toughness of the laminate as a whole. Obviously, the dissipated energy can be split in a part related to delamination and a part related to matrix cracking, such that the total dissipated energy $E$ is defined as

$$E = E_{\text{delamination}} + E_{\text{matrix}} = \int_{\Gamma_i} G_d \, d\Gamma + \int_{\Gamma_m} G_m \, d\Gamma$$ (3.23)

where $\Gamma_i$ is the surface domain of the interface between the plies, and $G_d$ and $G_m$ are the dissipation per unit area related to delamination and matrix cracking, respectively. For the plane stress interface elements with a single mode damage law,
the dissipation per unit area can be computed straightforwardly with

\[
G_d = G_{\text{H},d} \cdot \max_{\tau \leq t} \left\{ \begin{array}{l}
0, \quad [\hat{u}]_{\text{sh}} \leq [\hat{u}]^0_{\text{sh}} \\
\frac{[\hat{u}]_{\text{sh}}^0 - [\hat{u}]_{\text{sh}}}{[\hat{u}]^0_{\text{sh}} - [\hat{u}]_{\text{sh}}^0}, \quad [\hat{u}]_{\text{sh}}^0 < [\hat{u}]_{\text{sh}} < [\hat{u}]^f_{\text{sh}} \\
1, \quad [\hat{u}]_{\text{sh}} \geq [\hat{u}]^f_{\text{sh}}
\end{array} \right.
\] (3.24)

while numerical time integration is required to compute the dissipation in a mixed mode cohesive point related to matrix cracking. Euler backward integration gives for the local dissipation after time step \(n\):

\[
G_m = \sum_{i=1}^{n} \left( \kappa_{m,i} - \kappa_{m,i-1} \right) G_{T_c,i}(\alpha)
\] (3.25)

with \(\kappa_m\) from Equation (2.38), \(\kappa^f_m\) from Equation (2.46) and \(G_{T_c}\) from Equation (2.29).

In Figure 3.8 the dissipation at the end of all twelve analyses is visualized. Again, the results with Newton-Cotes integration prove to be converging to a unique solution very fast. The energy dissipation due to delamination in the analyses with Gauss integration decreases upon mesh refinement. The fact that more energy is dissipated before a mechanism is formed with Gauss integration can be well understood considering that the unadapted interface elements are bridging the splitting crack. Eventually, the interface is damaged on both sides of the crack, because in the unadapted interface element relative displacements become large over the whole element domain, while in the real discontinuous displacement field significant relative displacements occur on one side of the crack only. This is illustrated in Figure 3.9, showing the area with delamination damage and the location of the matrix cracks. It can be observed that with Gauss integration the final delamination front lies outside of the area bound by the splitting cracks, while with nodal integration, the delamination front lies, on average, on the cracks.
3.3 Crack spacing

It is concluded that unadapted interface elements can be used between elements that are cracking with the phantom node method without reservation. When unadapted interface elements are used, a nodal (Newton-Cotes) integration scheme is to be preferred because with such a scheme the displacement jump is exact in all integration points and no artificial bridging is introduced.

3.3 Crack spacing

In a mesolevel laminate model, the strains in different plies are necessarily matching until delamination takes place. Neglecting the out-of-plane shear deformation, the displacement field in the different plies is exactly the same as long as the interface is undamaged. Matrix cracks that are introduced as a discontinuity in the displacement field do not change this, except at sub-element level. In other words, introduction of transverse cracks after violation of the failure criterion does not necessarily lead to localization of deformation and hence to unloading of the surrounding material. This gives the stress based laminate analysis an ill-posed character. In absence of delamination the stress keeps increasing in every uncracked element. Eventually, the strength may be exceeded throughout the domain. With a rigid interface, the stress field may give rise to an infinite number of cohesive cracks with infinitesimal crack spacing.

Physically, the ill-posedness of the mechanical problem is reflected in the apparent randomness of the exact location of matrix cracks. The exact location of subsequently appearing matrix microcracks and the distance between those cracks...
depends on the microstructural fiber distribution and on the complex three-dimensional displacement field in the neighborhood of existing cracks. The resolution of the mesolevel model is by definition not sufficiently fine to capture this. However, this is not necessarily problematic, because in mesolevel analysis one is not really interested in finding the exact location of individual transverse cracks.

A statistical strength distribution could alleviate the ill-posedness in the sense that a unique location can be found where cracks should initiate first. But if these first cracks do not cause significant delamination, increasing strain may still lead to a theoretically infinite number of cracks, except when the full three-dimensional problem is solved with multiple elements over the ply thickness.

In the example in the previous section, the ill-posedness was removed by predefining where matrix cracks are allowed. As a consequence, the strength criterion was not applied consistently throughout the domain. There were areas where the stress exceeded the strength but where the material was nonetheless assumed to remain intact. However, the phantom node method can deal with multiple parallel cracks, provided that the number of these cracks is finite. Therefore a numerical crack spacing parameter is introduced to remove the ill-posedness while maintaining as much as possible the predictive quality that cracks may initiate wherever needed. Because the matrix cracks are straight, the normal distance between a pair of cracks can be computed, which is used as a limiter for crack initiation.

Another advantage of using a predefined minimum crack spacing is that this allows for the modeling of coalescing cracks. Since we are dealing with straight cracks it can be anticipated that two cracks will meet. Practically this means that crack initiation at a location with zero normal distance to an existing crack is also allowed.

The crack propagation/initiation procedure is implemented such, that whenever the matrix strength is exceeded in an element, the projected distance from this element to existing cracks is checked. If that distance is smaller than the predefined crack spacing, it is tried to move the point of initiation of the new crack inside
the failing element such that the two cracks will exactly meet. If that fails, crack
initiation in this element is aborted, and the same element will not be checked for
failure again. New crack segments are either an extension of an existing crack, or
the initiation of a new crack with $\Delta \geq \Delta_{\text{min}}$ or the initiation of a new crack that is
anticipated to meet an existing crack $\Delta = 0$ (see Figure 3.10). Initiation of cracks of
the last kind is particularly important for robustness. To understand this, consider
the elements in Figure 3.10 where initiation takes place with $\Delta = 0$. If initiation
would not be allowed here, the stress in these elements would start exceeding the
strength. Later, when the existing crack propagates through these elements, the
introduction of cohesive segments would be accompanied by a discontinuity in the
global response, because the initial traction which is equal to the strength is not in
equilibrium with the stress prior to failure. This causes a sudden drop in the nodal
forces which may lead to non-convergence. And once this happens, non-convergence
cannot be circumvented by reducing the step size.

It is not immediately clear how the value of $\Delta_{\text{min}}$ should be chosen. A lower bound
is related to the fineness of the mesh, practically because in our current implementa-
tion multiple cracks per element cannot be dealt with, and philosophically because
the fineness of the discretization indicates the desired resolution of the approxima-
tion. In this section, the influence of the crack spacing on the results is investigated
with two numerical examples, with emphasis on the question how this parameter
influences the objectivity of the global response.

**Nearly uniform strip** Firstly, an hourglass-shaped $[0/90]_s$ strip is considered. Two
plies are modeled, each discretized with 401 elements in longitudinal direction and
one element over the width. Poisson’s ratio is set to zero, such that the coarse
discretization in $y$-direction is justified.

The analysis is performed with different values for the crack spacing parameter.
The first crack in the $90^\circ$-ply appears in the element with the smallest width. As

![Figure 3.11 Number of cracks in strip analysis versus value of crack spacing parameter.](image)
the load increases further, more transverse cracks are initiated and some of them are eventually accompanied by delamination. The decohesion is completed only in those cracks from which delamination propagates. In absence of a representation of fiber failure, the 0°-ply remains elastic. The computations are terminated when \( u = 1 \text{ mm} \), at which stage there is a stable number of cracks that is monotonically opening with growing zones of delamination in between.

For each of the computations, the number of initiated cracks is counted as well as the number of cracks which are open. Here, we speak of open cracks when decohesion is complete. In Figure 3.11, these counts are compared with the total number of cracks that is allowed in the specimen, which is computed by dividing the specimen length over the crack spacing. It can be observed that if the spacing is small enough, the number of initiated cracks and the number of open cracks both converge to a unique value.

In Figure 3.12 the final energy dissipation due to matrix cracking and delamination is shown for different values of the crack spacing. For a spacing that is larger than 0.5 mm, the number of allowed cracks is smaller than the number open cracks in the limit case (see Figure 3.11). It is in these cases, that the dissipation depends strongly on the spacing parameter, although the influence on the total dissipation is still limited due to the opposite trends in matrix and delamination contributions. But if the number of open cracks is approximately correct (spacing \( \leq 0.5 \text{ mm} \)), the influence becomes small.

The fact that the number of cracks that is initiated is limited seemingly contradicts the introduction to this section. The problem is well-posed after all. This is due to the finite elastic stiffness of the interface, which was neglected before. The cracked transverse ply can be understood as an elastically supported slab as shown in Figure 3.13. After some initial opening of the crack, there exists a point with a finite distance from the crack at which the stress in the 90°-ply has a maximum. If the mesh is sufficiently fine and the crack spacing sufficiently small, the location
of the next crack will be given by this maximum rather than by the crack spacing. Therefore, in this simple case in which coalescence of cracks does not occur, the crack spacing parameter could even be set equal to zero. The objective spacing that is thus obtained depends largely on the elastic stiffness of the interface, which is itself not a particularly objective parameter. The elastic deformation of the interface can be understood as representing the deformation of the ply due to initial crack opening, which is indeed a physical process that prevents cracks from initiating too close to one another. Notably, in three dimensional analysis with a single element per ply in thickness direction, it is more appropriate to use a very high dummy stiffness in the interface, which will dramatically reduce the objective crack spacing.

The final displacement field obtained with different values for the spacing parameter is visualized in Figure 3.14, with the displacement jumps related to the opening cracks in the transverse plies clearly visible. These jumps are spaced regularly in the analyses with large crack spacing defined, because in those cases each of the allowed cracks is opening. The pattern is less regular but eventually becomes unique for decreasing crack spacing. The final irregular pattern is the result of the complex process in which the stress concentration in the interface near individual matrix cracks causes propagation of delamination and subsequently unloading of the surrounding material in the transverse ply and closing of neighboring matrix cracks.

That not all matrix cracks are accompanied by delamination when the spacing is small, can again be observed in Figure 3.15, where the matrix cracks and delamination damage are visualized for two values of the crack spacing. When the spacing is large, there is an isolated zone with delamination around every single matrix crack in the 90°-ply, whereas for small spacing the number of cracks is higher than the number of zones with delamination.
Chapter 3 Laminate analysis

Figure 3.14 Final deformation in strip analysis for different values of the crack spacing, visualizing the fully damaged cracks.

Figure 3.15 Matrix cracking and delamination in strip analysis with crack spacing of 0.75 mm (top) and 0.2 mm (bottom).

Open hole laminate  Secondly, the $[\pm 45]_s$ laminate with circular hole from the previous section (see Figure 3.4) is revisited. This time there are no predefined crack locations, and the number of cracks is limited by the spacing. Different values of the crack spacing parameter are used. For the computations with larger spacing ($\Delta x \geq 0.6$ mm) the mesh with approximately 4000 nodes per ply is used and for those with smaller spacing ($\Delta x \leq 0.5$ mm) the mesh with 8000 nodes per ply is used.

Peak load values are displayed in Figure 3.16. Two different plateaus where the maximum load is roughly constant can be observed. The cause for the drop in maximum load for ($\Delta x < 0.9$ mm) is found in subcritical delamination near the hole. In all computations, the first cracks are initiated at the same location along the hole, since the crack spacing does not influence the solution before any cracks are present. The location of these first cracks is at the point where the cross section is minimal. Then, as the load continues to increase, more cracks are initiated. In case the spacing is small enough to have secondary parallel cracks that also touch the circular hole, the small triangular areas that are enclosed by these cracks delaminate before the maximum load is reached (see Figure 3.17). The consequence of this
3.3 Crack spacing

The influence of the spacing on the final delaminated area can be observed in Figure 3.17, which depicts the final crack pattern and delaminated area for four different values of the crack spacing. Load-displacement diagrams are also shown. There is no absolutely unique solution, but a strong similarity between the results with different crack spacing values can nevertheless be observed.

Sharp snapback events are recorded when a matrix crack reaches the boundary and a fiber bundle is free to unload at once (see Figure 3.18). Neglecting dynamical effects for these events is not realistic, but simulation of such a dynamic event is far from trivial. The dissipation-based arclength method is a powerful technique to model such dynamic events in a robust and clean manner.

Notably, the fact that in this case the secondary cracks eventually form the main opening macrocracks, makes predictive analysis of the failure mechanism particularly challenging. With the present approach, this challenge can be met. The transition from the distributed phenomenon in a zone with parallel matrix cracks to the discrete phenomenon in which individual cracks from this zone become dominant is captured automatically as a consequence of proper ply kinematics and sound interaction between matrix cracking and delamination.

The influence of crack spacing on the final dissipation is shown in Figure 3.19. Here too, the influence of the presence of subcritical damage is visible, particularly in the dissipation related to delamination. For the dissipation in the matrix cracks, a completely unique response has not been obtained. But on the other hand, the influence of crack spacing on dissipation is limited, even when only dissipation due to matrix cracking is considered. Not all cracks that are initiated are fully opening, so the amount of energy that is dissipated in distributed matrix cracking is not linearly dependent on the number of cracks. That the response is not completely unique is in this case acceptable as a reflection of the fact that there is randomness in the

Figure 3.16 Peak load value for open hole laminate for different values of the crack spacing.
Figure 3.17 Load-displacement diagrams along with final delamination damage and matrix cracks for different values of the crack spacing.
3.3 Crack spacing

Figure 3.18 Deformation shortly before and after a sharp snapback. Deformations are scaled with a factor 10; the crack spacing is 0.6 mm; the ellipse indicates the region where failure progresses. During the snapback part of the top ply unloads after one of the matrix cracks has reached the boundary.

Figure 3.19 Energy dissipation for open hole laminate for different values of the crack spacing.

exact location of matrix cracks. No data was obtained for crack spacing of 0.9 mm, because in that computation the secondary cracks that only just missed the hole eventually caused difficulties in the post peak analysis.

It is concluded from both examples in this section that the artificial crack spacing parameter does not have a pathological influence on the results. When the spacing is chosen sufficiently small to describe the final delamination pattern, the predicted peak load value is largely independent of the value that is used for the spacing. The total dissipation, a quantity strongly related to the the post-peak response, remains more sensitive to this value, but not to such an extent that the amount of energy dissipated in the matrix cracks is inversely proportional to the spacing. The optimal value for the spacing parameter remains problem and mesh-dependent, but with this approach it is possible to deal with both distributed matrix cracking and discrete splitting, and to have a transition between the two, which is governed by the mechanics in the interface as it should be.
3.4 Plane stress approach

To this point, all laminate analyses have been performed in plane stress. In this plane stress approach out-of-plane coordinates do not exist and out-of-plane displacements are not solved. Nevertheless, through-thickness variations are present because each ply is modeled with a separate layer of elements. The tractions in the interface elements between the plies are the $\tau_{zx}$ and $\tau_{zy}$ stress components, which are normally absent in plane stress analysis.

One limitation of the plane stress approach can already be identified before performing any computations. Namely that the possible influence of mirroring the ply stacking sequence of the halves of a symmetric laminate will never be captured. In the plane stress approach, no distinction is possible between $[0/90]_s$ and $[90/0]_s$ layups, because the symmetry condition is necessarily treated exactly the same as the surface boundary condition.

In this section, the validity of the plane stress approach is examined. The analysis of a plate with a hole is revisited with two issues of concern in mind. The first question is whether neglecting out-of-plane deformation and hence mode I opening of the delamination crack influences the response. The second question is about the influence of the elastic interface stiffness on the results. This is an additional parameter in the plane stress analyses.

Open hole laminate

Firstly, the open hole analysis with nodal integration from Section 3.2 is repeated in 3D. For this purpose, the mesh with approximately 2000 nodes is extruded such that each ply is represented with a layer of 6-node prismatic elements. Obviously, with one layer of elements per ply, the three dimensional stress state is still not resolved accurately, but Jiang et al. [50] have shown that increasing the number of elements in thickness direction has only limited effect on the global solution for similar analyses. In the three-dimensional analysis, a high value of $K_d = 10^8$ N/mm$^3$ is used in the interface elements (recall that in the two-dimensional analysis it was equal to $K_d = G_{12}/(t/2) = 22 \cdot 10^3$ N/mm$^3$). Furthermore, $v_{23}$ is set to 0.4, and for the other out-of-plane elastic parameters transverse isotropy is assumed. Secondly, the 2D analysis is repeated with the same mesh, while varying the value for the elastic interface stiffness $K_d$.

In Figure 3.20 the load-displacement response from the three-dimensional and plane stress analysis are compared. Strikingly, the curves are practically on top of each other. Except for small deviations at the two major peaks, there is no visible difference between the plane stress and the three-dimensional response. There is a small difference in maximum load (1.70 kN versus 1.74 kN) as well as in total dissipation (82.5 Nmm for 3D versus 84.3 Nmm for plane stress). The latter difference is due to the fact that delamination in the three-dimensional analysis had a mixed
mode character; the nonzero normal component of the displacement jump causes a decrease in energy dissipation in the interface (note that $G_{Ic} \leq G_c \leq G_{IIc}$ while in plane stress $G_c \equiv G_{IIc}$). The same fact is likely to have an influence on the peak load, since the peak load is related to propagation of delamination and hence to the delamination fracture energy. However, the difference in peak load value is also influenced by the elastic deformation of the interface, which is not an exact representation of the out-of-plane shear deformation of the solids.

This is illustrated by the results from the series of simulations with different values for $K_d$ as shown in Figure 3.21. Varying the elastic interface stiffness does not influence the total energy dissipation, since the failure mechanism is in all cases the same. But the influence on the peak load value is significant. For high values of the interface strength, the peak load approaches a limit value. But if the three-dimensional solution is taken as a reference, the limit value is not correct. This confirms the idea that it is appropriate to allow for finite elastic deformation of the interface in plane stress analysis. It is reasonable to relate the value of the stiffness to the ply thickness $t$ and the shear stiffness $G_{12}$ or $G_{23}$. In the current example, very good agreement is reached with $K_d = 16.5 \cdot 10^3 \text{N/mm}^3$, which corresponds with $G_{12}/(\frac{3}{4}t)$. But the value for which optimal agreement exists is likely to be problem dependent.

It is concluded that the plane stress approach is attractive as an efficient and robust approach that provides relevant insight in the failure process. In laminate failure analysis under tensile loading, the most important processes are captured without solving the out-of-plane displacement field. Choosing a finite elastic stiffness for the interface gives better agreement with three-dimensional results than giving it a very high dummy value, but the exact value does influence the solution. Since the elastic deformation of the interface represents out-of-plane shear deformation of the ply, it should be related to the thickness and the shear stiffness of the ply.
Figure 3.21 Influence of elastic interface stiffness in plane stress analysis on open hole laminate failure characteristics, in comparison with values from 3D analysis.
Chapter 4 Solution procedure

In the previous two chapters, a numerical framework for the simulation of composites has been introduced, first for the single ply and then for a complete laminate. However, carefully constructed kinematic and constitutive models are not all that is needed for successful simulations. When the computation crashes due to non-convergence before the virtual specimen has failed, the model is of no use. And when the computation time is very high this does not encourage its use either. In order to get the model working in complex cases, a well-designed solution procedure is indispensable. The key targets in formulating this procedure are robustness and efficiency.

The presented model has several aspects that complicate the solution procedure. Firstly, sharp snapbacks are encountered (see e.g. Figure 3.17). When matrix failure occurs in fibrous materials, two processes take place simultaneously: matrix material damages (by definition), and fibers unload (as a possible consequence). Because the fibers are very stiff and the matrix failure process is not very ductile, the amount of elastic energy released by the second process easily exceeds the amount of energy necessary to drive the first. Hence, damage grows in an unstable manner and snapback behavior is observed in the equilibrium path. The failure process can therefore not be simulated with a monotonically increasing prescribed displacement at the loaded boundary. There is no equilibrium solution for such boundary conditions. Therefore, an arclength method must be employed, which can follow the equilibrium path through a snapback. In this work, the dissipation-based method by Gutiérrez [31] is used. The method will be outlined in Section 4.1, along with an extension of the formulation that is needed with the proposed constitutive models.

Secondly, the initiation and propagation of cracks with the phantom node method must be given a place in the solution procedure. This is a remeshing operation that is not suitable for integration in the Newton-Raphson procedure. However, due to the possibility of distributed cracking, many cracks can be expected, which should be dealt with as efficiently as possible. The strategy for crack propagation will be presented in Section 4.2.

Thirdly, an adaptive time stepping strategy is needed. In laminate fracture, different failure processes may occur and interact. In some cases the different processes are competing, in other cases they promote one another, but in either case the system is highly nonlinear. When failure first occurs in a distributed fashion and then starts localizing, the material switches from loading to unloading in part of the do-
main. At a later stage the loading may continue. When such things happen, it is not certain that the Newton-Raphson procedure will find the solution, even if exact linearization is consistently applied. Therefore, an adaptive strategy is implemented, which searches for an increment size for which the Newton-Raphson procedure does converge. The adaptive strategy will be presented in Section 4.3.

Fourthly, the fiber failure model gives particular convergence problems which cannot be solved with adaptive time stepping. Therefore, a modified Newton-Raphson scheme is used in some cases when the fully linearized iterative procedure does not converge. In Section 4.4 it will be explained how and when this is done.

### 4.1 Dissipation-based arclength method

The material models described in the previous chapters are embedded in an implicit quasi-static finite element framework. The equilibrium path is followed with the dissipation-based arclength method, which was developed by Gutiérrez [31]. Like with other arclength methods, a constraint equation is added to the system of equations. In the dissipation-based arclength method, the constraint equation is based on the thermodynamical principle that energy dissipation is non-negative in each finite time increment. With this in mind, a forward marching strategy along the equilibrium path is defined by prescribing a finite amount of energy to be dissipated in each time step. In Figure 4.1, it is shown how the equilibrium path is followed incrementally with equal energy increments. In contrast with other robust arclength methods for modeling of failure, the constraint equation is defined in terms of global quantities, and therefore, there is no need to prescribe or track where the localized deformation occurs.

**Original formulation** In the dissipation-based arclength method, the constraint equation is formulated such that an increment in the energy dissipation is prescribed in each time step. For models with secant unloading, the constraint equation is

\[
F_u^a = \frac{1}{a_i - 1} \Delta E_i
\]

Equilibrium path with snapback

**Figure 4.1** Incremental solution of equilibrium path with a snap back with the dissipation-based arclength method. The energy dissipation per time step is prescribed.
4.1 Dissipation-based arc-length method

expressed in terms of nodal quantities as:

\[
\frac{1}{2} \hat{\mathbf{f}}^T (\lambda_0 \Delta \mathbf{a} - \Delta \lambda \mathbf{a}_0) = \Delta E
\]

where \( \hat{\mathbf{f}} \) is the unit load vector, \( \lambda \) is the load scale factor (\( \lambda \hat{\mathbf{f}} = \mathbf{f}^{\text{ext}} \)), \( \mathbf{a} \) is the nodal displacement vector, and \( \Delta E \) is the prescribed amount of dissipated energy in the time step. The subscript 0 is used to refer to a quantity at the beginning of the time step, while \( \Delta \) indicates an increment during the time step.

In the left diagram of Figure 4.2, the quantities from Equation (4.1) are illustrated for a single degree of freedom. Assuming the path between the two points on the load-displacement curve is straight, the area \( \Delta E \) can be expressed as

\[
\Delta E = \frac{1}{2} (\lambda_0 \Delta u - \Delta \lambda u_0)
\]

which is strongly similar to the generalized form in Equation (4.1). However, it is obvious from the figure that this expression depends on the assumption of secant unloading. In case permanent deformations are present, the constraint equation has to be adapted.

**Damage/plasticity formulation**  In the analysis of laminate failure with the proposed framework, the assumption of secant unloading does not hold for two reasons, firstly due to the residual stress from the curing process (see Section 1.5), and secondly due to the permanent strain related to shear nonlinearity (see Section 2.6). An extension to plasticity has been derived before by Verhoosel et al. [128]. In that derivation, however, it is tacitly assumed that plasticity is the only dissipative mechanism, which is not the case in our model. Therefore a new constraint equation is derived below that is generic for combined damage and plasticity.

Following Gutiérrez [31], the dissipation rate \( G \) is computed as the difference
between the exerted power $P$ and the rate of elastic energy $\dot{V}$:

$$\dot{E} = P - \dot{V}$$  \hspace{1cm} (4.3)$$

with

$$P = \lambda \dot{a}^T \hat{f}$$  \hspace{1cm} (4.4)$$

where $\hat{f}$ is a unit load vector, $\lambda$ is the load scale factor and $\dot{a}$ is the nodal displacement rate.

The elastic energy $V$ is defined as

$$V = \frac{1}{2} \int_\Omega (\varepsilon - \varepsilon^p - \varepsilon^{th})^T \sigma \, d\Omega + \frac{1}{2} \int_\Gamma [\mathbf{u}]^T \mathbf{t} \, d\Gamma$$  \hspace{1cm} (4.5)$$

where $\Omega$ is the bulk domain and $\Gamma$ is the cohesive surface, either in an interface element or in a phantom node crack. With the kinematic relations $\varepsilon = \mathbf{B} \dot{a}$ and $[\mathbf{u}] = \mathbf{Z} \dot{a}$, this can be reorganized to

$$V = \frac{1}{2} \dot{a}^T \left( \int_\Omega \mathbf{B}^T \sigma \, d\Omega + \int_\Gamma \mathbf{Z}^T \mathbf{t} \, d\Gamma \right) - \frac{1}{2} \int_\Omega (\varepsilon^p + \varepsilon^{th})^T \sigma \, d\Omega$$  \hspace{1cm} (4.6)$$

The two integral terms between parentheses can be eliminated, because they are equal to the internal force vector, and hence, when equilibrium is satisfied, to the external force vector. So the elastic energy is rewritten as

$$V = \frac{1}{2} \lambda \dot{a}^T \hat{f} - \frac{1}{2} \int_\Omega (\varepsilon^p + \varepsilon^{th})^T \sigma \, d\Omega$$  \hspace{1cm} (4.7)$$

Note that the integral with the operator $\mathbf{Z}$ has been eliminated without specifying whether this signifies the kinematic relation in an interface element or in a pair of elements with the phantom node method. However, secant unloading in the cohesive zone has been assumed in Equation (4.5).

With Equation (4.7), assuming constant $\varepsilon^{th}$, the rate in elastic energy is:

$$\dot{V} = \frac{1}{2} \left( \dot{\lambda} \dot{a}^T \hat{f} + \lambda \ddot{a}^T \hat{f} \right) - \frac{1}{2} \int_\Omega (\dot{\varepsilon}^p)^T \sigma + \ddot{\sigma}^T (\varepsilon^p + \varepsilon^{th}) \, d\Omega$$  \hspace{1cm} (4.8)$$

After substitution of $\dot{\varepsilon}^p = \mathbf{F} \dot{\mathbf{B}} \dot{a}$ and $\ddot{\sigma}^p = \mathbf{D} \dot{\mathbf{B}} \dot{a}$ this can be reorganized to

$$\dot{V} = \frac{1}{2} \left( \dot{\lambda} \dot{a}^T \hat{f} + \lambda \ddot{a}^T \hat{f} - \dot{a}^T \mathbf{f}^* \right)$$  \hspace{1cm} (4.9)$$

with

$$\mathbf{f}^* = \int_\Omega \mathbf{B}^T \mathbf{F}^T \sigma + \mathbf{B}^T \mathbf{D}^T (\varepsilon^p + \varepsilon^{th}) \, d\Omega$$  \hspace{1cm} (4.10)$$
where $\mathbf{D}$ is the consistent tangent matrix $D_{ij} = \partial \sigma_i / \partial \varepsilon_j$ and $\mathbf{F}$ is the gradient of plastic strain with respect to total strain $F_{ij} = \partial \varepsilon_p^p / \partial \varepsilon_j$.

Substitution of (4.4) and (4.9) into Equation (4.3) gives

$$\dot{\mathbf{E}} = \frac{1}{2} \left( \dot{\mathbf{a}}^T \left( \lambda \dot{\mathbf{f}} + \mathbf{f}^* \right) - \lambda \dot{\mathbf{a}}^T \dot{\mathbf{f}} \right)$$  \hspace{1cm} (4.11)

With forward Euler integration we arrive at the constraint equation, which prescribes that a finite amount of energy, $\Delta E$, is dissipated in the time step

$$\frac{1}{2} \left( \lambda_0 \Delta \mathbf{a}^T \dot{\mathbf{f}} - \Delta \lambda \mathbf{a}_0^T \dot{\mathbf{f}} + \Delta \mathbf{a}^T \mathbf{f}^* \right) = \Delta E$$  \hspace{1cm} (4.12)

The first two terms are equal to the left hand side of the original form in Equation (4.1). The third term is new and asks for the assembly of an additional vector. Due to the forward Euler integration, the vector $\mathbf{f}^*$ has to be evaluated only at the beginning of the time step. However, when the discretization changes due to crack growth with the phantom node method, it has to be re-evaluated.

### 4.2 Crack growth

In Section 2.2, it has been proposed to use the phantom node method for matrix cracking. The method has been adopted in this work to model problems with initiation and propagation of cracks, possibly many of them. In this section, it is presented how the crack growth is handled in the solution procedure.

**Position in global algorithm** In partition of unity-based methods, crack growth is dealt with outside of the Newton-Raphson loop. Doing it inside the Newton-Raphson loop either implies that the cracks may grow based on a non-equilibrium solution, which is physically unsound, or it requires that crack growth is reversible inside the Newton-Raphson loop, which harms the robustness of the solution procedure.

Therefore, the stress field is checked for failure after an equilibrium solution has been found. Together with the adaptive stepping, this results in a solution algorithm for the single time step with a threefold loop (see Figure 4.3). The innermost loop is the Newton-Raphson loop, which is standard for nonlinear finite element computations. In step $\{1\}$, the new solution vector is initialized to be equal to that from the previous time step, and the boundary conditions are updated. In step $\{2\}$, the residual vector, is updated for the current displacement field, where the residual is the unbalance in the weak form of the equilibrium equation, cf. Equation (1.1):

$$\mathbf{r} = \mathbf{f}^{\text{int}}(\mathbf{a}) - \mathbf{f}^{\text{ext}}$$  \hspace{1cm} (4.13)
In step \{3\}, the relative magnitude of this unbalance $R$ is computed, and it is checked whether this is small enough to consider the current displacement field an equilibrium solution. The criterion for this is:

$$R = \frac{||r||}{||r||_0} < R_{\text{min}}$$

(4.14)

Where $||r||_0$ is the norm of the residual vector from the first iteration. As long as the criterion (4.14) is not satisfied, the system is repeatedly linearized and solved with Equation (1.10) in step \{5\}, but not before in step \{4\} it has been checked whether there is still hope that the Newton-Raphson procedure will converge. If the residual becomes too high ($R > R_{\text{max}}$) or the number of iterations too large ($n > n_{\text{max}}$), the procedure is canceled and restarted with a new increment (see Section 4.3).

After an equilibrium solution has been found, the corresponding stress field is checked for failure in step \{6\}. The solution is acceptable if the failure criterion is not violated in any of the elements where cracking is allowed. Then the solution is stored (history is updated, output is written, etc.) in step \{8\}. In contrast, when the failure criterion is violated, new cracks segments are inserted, either as growth of existing cracks or as initiation of new cracks. This is basically a remeshing operation: the discretization of the displacement field is changed. After this, equilibrium is no longer satisfied. There are three options for how to continue: proceed to the next time step (\{7\}→\{8\}), restart the current time step (\{7\}→\{1\}), or continue the Newton-Raphson loop (\{7\}→\{2\}). The third option is to be preferred, which will be argued below.
4.2 Crack growth

As long as time steps are sufficiently small, it can still be assumed that the solution before crack growth is close to the real solution path, since with cohesive tractions the perturbation of the equilibrium is small. Therefore, one might be inclined to proceed to the next time step directly after crack growth, like Wells and Sluys [132]. This would be most efficient, and the small loss in accuracy could be acceptable. However, even the loss in accuracy is accepted regarding the gain in efficiency, robustness requires otherwise. It is possible that the Newton-Raphson scheme does not converge after crack growth. If we would then proceed to the next time step, step size reduction in that step will be of no avail. The simulation will crash irrevocably, unless a more complicated adaptive scheme is implemented which can go back to the beginning of the previous time step. Therefore, the option to go from step \{7\} directly to step \{8\} is discarded. It is necessary to find equilibrium again before the solution is committed. In that case, if no convergence is found after crack growth, we are still in the same time step and crack growth can be canceled (in step \{9\}) to go back to the beginning of the time step with a different increment (see Section 4.3). The next time step is entered if and only if a solution has been found that satisfies both equilibrium and the failure criterion.

In a given finite element implementation, it can be more straightforward to restart the time step at \{1\} than to continue with the converged but not-accepted solution at \{2\}. For efficiency, however, it is to be preferred to re-enter the Newton-Raphson loop with the latest converged solution. This displacement field, which satisfies equilibrium as well as the constraints for this time step, gives a better estimate for the final solution of the time step (see Figure 4.4, \(a_{1}^{0}\) is closer to \(a_{i}\) than \(a_{i-1}\)). Using the latest converged solution reduces the number of iterations needed to re-establish equilibrium considerably. This is especially advantageous when the crack growth loop is passed several times inside a time step.
Crack growth procedure It is crucial for efficiency that it is possible to introduce multiple new crack segments before the iteration loop is entered again. The computation would become unnecessarily lengthy if equilibrium were sought again after each propagation through a single element. The procedure for crack growth in steps \{6\} and \{7\} is illustrated in more detail in Figure 4.5. First, the stress is checked in all integration points in all elements where failure is allowed. The values from the failure criterion evolution are sorted in descending order and stored per ply. Then, crack segments are introduced element by element, beginning with the element with the highest violation. After each initiation of a new crack, the set of elements in which cracking is allowed is updated, considering the restrictions related to the crack spacing (see Section 3.3). New segments are introduced until no more elements exist in which the failure criterion is violated and in which cracking is allowed or until a maximum number of new crack segments per ply has been reached.

**Figure 4.5** Algorithm for crack growth with possibly multiple new crack segments before re-entering the Newton-Raphson loop (for the location in the full procedure, see Figure 4.3).

With the irreversibility of crack growth, this may in some cases cause cracks to be initiated or extended too fast. It is possible that crack growth in one place would reduce the stress elsewhere if equilibrium were re-established, and that further crack growth should therefore not take place, while it does in the proposed strategy. But generally, this is not the case because crack growth at one place rather tends to cause stress to increase elsewhere. We have found no significant influence on the results when the maximum number of simultaneously inserted new crack segments was increased from 1 to 200 per ply. At the same time, this increase effectuates a dramatic reduction of the computation costs in cases with many cracks.

Verhoosel [129] argues that only one crack segment should be allowed per time step. This comment is not substantiated in his thesis, and from the considerations above, it follows clearly that the advise is not followed in this work.
4.3 Adaptive increment strategy

For the convergence of the iterative procedure, it is important that the new degrees of freedom are initialized at values that are close to their unknown final values. With the phantom node method, a very good estimate can be made by equating the displacements of a new phantom node to those of the corresponding original node. This results in a zero displacement jump in the new crack segment, and therefore to a displacement field that is optimally close to the last converged solution.

4.3 Adaptive increment strategy

Because laminate failure is constituted by a series of relatively brittle failure events, it is a challenge to design a loading strategy with which the capricious equilibrium path can be followed. The dissipation-based arclength method is a very powerful tool for this purpose. However, this method does not guarantee that a solution will always be found. A single case of non-convergence should not lead to termination of the computation, because it is very well possible that for another increment size, the analysis may be continued. Therefore, a strategy that is adaptive with respect to the increment size is necessary.

Furthermore, the dissipation-based arclength method only works when energy is actually being dissipated. When the system is completely elastic, the system of equations with the additional constraint equation becomes singular. Therefore a hybrid loading strategy is used which uses standard displacement increments in the initial stage and possibly again in later stages when no damage occurs. In short, both the size of the increment and its type (energy or displacement) are variable during the analysis.

In Figure 4.6, the algorithmic treatment of the possible increment changes is illustrated. The step numbers correspond with the numbering in the visualization of the global algorithm in Figure 4.3, although several new steps have been inserted that were left out before, viz. steps \{10\} to \{13\}. The dotted and dashed arrows correspond with the two loops with the same line types in Figure 4.3. The Newton-Raphson loop, however, is collapsed into a single box. The algorithm is presented in a different configuration with all arrows pointing downward to emphasize the implementation structure where we always go from one instance of the Newton-Raphson procedure via a possible change in the increment to the next instance of the Newton-Raphson procedure. Figure 4.6W is about what happens between these two instances of the iterative procedure.

During each instance of the Newton-Raphson procedure, the increment is fixed. But after it has been left, be it with convergence to step \{6\} or with non-convergence to step \{9\}, adaptation of the increment is possible. Especially in case of non-convergence many different actions may follow. In steps \{9a\} to \{9f\}, six different changes to the increment are possible. They are tried in the presented order until
Chapter 4 Solution procedure

Figure 4.6 Detailed algorithm for change in increment size or switch of increment type between two instances of the Newton-Raphson procedure (cf. Figure 4.3).

one of them succeeds. As soon as one succeeds, possible crack growth during this time step is canceled in step {9g} and the iterative procedure is restarted with the new increment. If none of the six changes can be applied, this means that we are out of options for finding a proper increment for this time step, and the computation is terminated. The order of the steps {9a} to {9f} is such that infinite loops and premature terminations are avoided.

The meaning of the steps {9a} to {9f} as well as of the newly inserted steps {10} to {13} will be explained in the remainder of this section.

Change in increment size The size of the increment can be changed following three different rules, depending on the outcome of the Newton-Raphson procedure and on the history of tried increments in this time step.

{11} At the end of the time step, i.e. when an equilibrium solution has been found that does not violate the failure criterion, the size of the increment is adapted according to

\[
\text{increment} \leftarrow 2^{-z} \cdot \text{increment}, \quad z = (n - n^{opt})/4
\]  

(4.15)

where \(n^{opt}\) is the optimum number of iterations. This is done irrespective of the type of increments that is used, energy or displacement. In case of crack growth, the number of iterations used in this expression, \(n\), is the maximum number of iterations in a single cycle of the Newton-Raphson procedure; the counter is reset each time equilibrium is reached but its maximum value during
the time step is used for the step size adaptation. Lower and upper bounds are
given for both energy and displacement increments. If \( n = n^{\text{opt}} \) the increment
size remains unchanged.

{9c} When convergence has not been reached, it often helps to reduce the size of
the increment. In step 9c, this is tried with a constant reduction factor \( c \):

\[
\text{increment} \leftarrow c \cdot \text{increment}
\]  

(4.16)

The lower bounds that are enforced in step 11 are again taken into account.
When the increment size is already below this lower bound, the reduction fails
and we proceed to step 9d

{9e} In exceptional cases it happens that a very small increment does not lead
to convergence, and that the difficulties can be overcome by taking a larger
increment. Therefore, when small increments of both types have been tried
without success, it is tried to increase the increment size. This is only done
with the generally more robust energy increments. The highest value that has
been tried in this time step divided by the reduction factor in Equation (4.16)

\[
\text{increment} \leftarrow \frac{1}{c} \cdot \text{increment}
\]  

(4.17)

The increase fails if the largest tried increment already exceeds the upper bound
\( \Delta E_{\text{max}} \).

**Switch of increment type**  
The type of the increment (displacement or energy) can be changed on different occasions. Obviously, compatibility of the boundary
conditions when switching from one type to the other is important. This is not au-
tomatically ensured, because the dissipation-based arclength method is based on a
scalable external force vector rather than on scalable displacements. The additional
unknown \( \lambda \) in the constraint equation (4.12) is a scale factor for the load vector. It
is only compatible with displacement control when nonzero displacements are pre-
scribed on a single degree of freedom, in which case the external force vector contains
only one scalable value. But it is possible to obtain compatibility with prescribed
displacements on a group of nodes, namely by adding node to node constraints for
all the nodes of that group and applying an external force on one of them.

The places where a switch from one type to the other can be made are listed below:

{10} A switch to energy increments is possible after convergence has been reached.
This switch is intended to be made at least once per analysis, because the analy-
sis always starts with displacement increments. For this purpose, the dissipated
energy is computed after convergence has been obtained with the standard non-
linear solver. If this exceeds a threshold value

$$\Delta E > \Delta E^{\text{crit}}$$ (4.18)

the switch to arclength control is made. Notably, this can happen in the middle
of the time step, i.e. before crack growth.

\{9a\} It is possible that at the low point of a snapback, the test specimen becomes
completely or almost completely elastic. This state is reached with energy in-
crements, but can be left only with displacement increments. In this case, it is
a waste of resources to go through a whole series of increment reductions before
the switch to displacement increments is made. Fortunately, this state can be
detected very efficiently in the first iteration that is done with the arclength
method. In the first iteration with an energy increment, the sca-
led residual is
evaluated with an additional check. If there is a large increase

$$R > R^{\text{crit}}$$ (4.19)

this is taken as an indication that the system is elastic, and the Newton-
Raphson procedure is aborted straight away with a message that is caught
in step \{9a\} and the switch to displacement increments is made. A flag is
set, indicating that this type of switch has been made. This flag disallows any
switching back to energy increments until step \{9f\} is reached.

\{12\} In highly nonlinear computations, sometimes very small increments are neces-
sary to find equilibrium. Unfortunately, the combination of the dissipation-
based arclength method with very small increments on the one hand and
remeshing with the phantom node method on the other can be problematic.
The reason for this is that upon remeshing, the stiffness of the numerical model
changes slightly. Typically, adding degrees of freedom makes the structure more
compliant. Because the remeshing occurs at a nonzero load level, this stiffness
reduction leads to spurious energy dissipation. If the mesh is sufficiently fine,
this change is negligible for the global response. But for very small energy incre-
ments it is possible that the spurious dissipation is larger than the prescribed
value, in which case the constraint equation can only be satisfied by global
unloading. A spurious snapback is the result. This is bad for efficiency, because
the model has to be reloaded carefully, and it possibly endangers robustness.
Therefore, it can be useful to fix the displacement increment after crack growth
for the remainder of the time step. This is especially the case when a mesh is
used that is relatively coarse. This switch is made after crack propagation when
the energy increment is smaller than $\Delta E^{\text{crit}}$. 
The switch to displacement control at step \{12\} has to be made undone at the end of the time step. This is done in step \{13\}. Notably, a jump in energy increment can be made, because the final amount of dissipated energy from this time step (after crack growth with fixed displacement) is used as the next increment.

When no convergence is reached after this temporary switch to displacement control has been made, the step is retried with the original energy increment, but with a flag that the switch at \{12\} is not allowed.

A switch from one increment type to the other is tried when reduction of the increment of the current type in step \{9c\} fails. After a switch to displacement control, the increment is set to the initial value $\Delta u^0$; after a switch to energy increments, it is set to the value from the last successful Newton-Raphson procedure. The switch to displacement control fails if the smallest allowed displacement increment has already been tried in this time step; the switch to energy increments fails if both the smallest and the largest allowed values have already been tried.

Finally, in exceptional cases it is possible that the switch in step \{9a\} has been made for while it should not be. In case no displacement increment has been found for which convergence could be attained after this switch has been made, we go back to energy increments in the hope that an energy increment size exists for which the Newton-Raphson procedure does converge. Obviously, the switch in \{9a\} is then disallowed for the remainder of the time step. This step fails if it is passed for a second time or if it is passed when the switch in step \{9a\} has not been made.

If the complete series \{9a\}–\{9f\} fails, this means that all possible increment sizes of both types have been tried. It is then and only then that the computation is terminated due to non-convergence.

Several tuning parameters have been introduced in this chapter. Optimum values for all of these are to some extent problem dependent, particularly those that are not dimensionless. A good set of values that has been used for all open hole tests in Section 5.2 is presented in Table 4.1. The different values that have been used for all analyses in this thesis are close to these values.

**4.4 Modified Newton-Raphson method**

The continuum damage model for fiber failure introduced in Section 2.5 with regularization according to the crack band method gives particular convergence problems.
Chapter 4 Solution procedure

Table 4.1 Algorithmic parameters as used in the open hole simulations in Section 5.2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optimal number of iterations</td>
<td>$n^{\text{opt}}$</td>
<td>6</td>
</tr>
<tr>
<td>Maximum number of iterations</td>
<td>$n^{\text{max}}$</td>
<td>10</td>
</tr>
<tr>
<td>Convergence criterion</td>
<td>$R^{\text{min}}$</td>
<td>$10^6$</td>
</tr>
<tr>
<td>Divergence criterion</td>
<td>$R^{\text{max}}$</td>
<td>$10^4$</td>
</tr>
<tr>
<td>Criterion for linear system</td>
<td>$R^{\text{crit}}$</td>
<td>10</td>
</tr>
<tr>
<td>Increment reduction factor</td>
<td>$c$</td>
<td>0.3</td>
</tr>
<tr>
<td>Critical energy dissipation</td>
<td>$\Delta E^{\text{crit}}$</td>
<td>0.1 Nmm</td>
</tr>
<tr>
<td>Maximum energy increment</td>
<td>$\Delta E^{\text{max}}$</td>
<td>10 Nmm</td>
</tr>
<tr>
<td>Minimum energy increment</td>
<td>$\Delta E^{\text{min}}$</td>
<td>$10^{-4}$ Nmm</td>
</tr>
<tr>
<td>Maximum displacement increment</td>
<td>$\Delta u^0$</td>
<td>0.01 mm</td>
</tr>
<tr>
<td>Minimum displacement increment</td>
<td>$\Delta u^{\text{min}}$</td>
<td>0.002 mm</td>
</tr>
</tbody>
</table>

Presumably this is due to difficulties that the Newton-Raphson procedure may have in finding a single band of elements that is damaging. This particular kind of ill-convergence manifests itself in an oscillatory response. The algorithm switches back and forth between two different solutions. The solution converges not to an equilibrium solution but to an oscillatory response, for which it holds that

$$K(a_i)^{-1}f^{\text{int}}(a_i) = -K(a_i-1)f^{\text{int}}(a_i)$$ (4.20)

Unfortunately, when this behavior is encountered, step size reduction is not effective.

Therefore a modified Newton-Raphson procedure has been implemented for this case, in which a partially secant matrix is used for $K$ instead of the fully linearized $K = \partial f^{\text{int}} / \partial a$. Inside the Newton-Raphson loop a check for oscillations in the residual norm is incorporated in step {3}. When oscillations are encountered, it is tried to escape these by using a not completely consistent tangent matrix. In a select set of integration points, the secant stiffness is used. For this purpose, the loading/unloading state of all material points is compared in each iteration with that from the previous iteration. In every point where the state changes from loading to unloading or vice versa, the secant stiffness is used in the subsequent iterations. Generally, this leads to an initial increase in the residual, but after several iterations the residual starts decreasing and the procedure converges slowly to the equilibrium solution. The maximum number of iterations is increased. When the residual norm decreases in 10 subsequent iterations, this is taken as an indication that the radius of convergence of the Newton-Raphson procedure has been reached. Then, the special strategy is terminated and consistent linearization is used again, often resulting in convergence in few additional iterations.

This is a rather costly and pragmatic technique, but it sometimes works to get beyond a critical point in the equilibrium path, which would otherwise only be passed after a long series of increment changes, if at all. This partially secant method is only performed when energy increments are applied.
Chapter 5 Validation

In this chapter, the numerical model for laminate failure presented in the Chapters 2 and 3 with the solution algorithm from Chapter 4 is tested. The numerical results are compared with experimental observations in order to validate the model. Furthermore, the sensitivity of the results with respect to different model parameters is investigated to increase the understanding of laminate failure and also to demonstrate the importance of modeling it.

Three cases are analyzed. Firstly, a notched plate with reference to experiments by Spearing and Beaumont [115, 116], secondly, the open hole tensile tests by Green et al. [29], and thirdly, the overheight compact tension test by Li et al. [65].

5.1 Notched plate

The first validation example is a \([90/0]_s\) laminate with a central notch is analyzed, which has been investigated experimentally by Spearing and Beaumont [115] and numerically by Wisnom and Chang [136]. The geometry and material parameters are given in Figure 5.1 and Table 5.1. Most parameters are from Spearing and Beaumont [115] and Wisnom and Chang [136]; the heat expansion coefficients are taken from Jiang et al. [50]; and shear nonlinearity parameters are chosen to fit data reported by Lafarie-Frenot and Touchard [57]. The minimum spacing between the matrix cracks is 0.5 mm. In all plane stress analyses in this chapter, the elastic stiffness of the interface depends on the ply thickness and is related to the in-plane shear stiffness with \(K_{12} = G_{12}/t\).

For composite laminates, it is often recommended to use \textit{in situ} parameters for the transverse strength. \textit{In situ} strength parameters take into account the fact that appearance of transverse matrix cracks does not only depend on the stress level, but also on the ply thickness and on whether the considered ply is an outer ply or

| Table 5.1 Material parameters used in notched plate analysis. |
|---------------------------------|----------------|----------------|----------------|
| Elasticity | Matrix/Delamination | Fiber failure | Shear nonlinearity |
| E_1 | 135 GPa | F_2s | 60 MPa | G_{11} | 1673 MPa | \(C_1\) | 22 |
| E_2 | 9.6 GPa | F_{12} | 75 MPa | G_{12} | 50 N/mm | \(C_2\) | -22 |
| G_{12} | 5.8 GPa | G_{12,e} | 0.15 N/mm | G_{12,m} | 0.4 N/mm | \(C_3\) | 35 |
| \(\nu_{21}\) | 0.31 | \(\eta\) | 1 | \(\alpha_1\) | 0 °C^{-1} | \(C_4\) | -5 |
| \(\nu_{23}\) | 0.4 | | | \(\alpha_2\) | \(3 \cdot 10^{-5} \) °C^{-1} | |
an inner ply [90]. Different analytical models are available that relate the strength to the ply thickness based on notions from linear elastic fracture mechanics (see e.g. Camanho et al. [14]). Here however, a cohesive crack approach is adopted, in which case the use of in situ strength is less obvious than in the simpler ply discount method (see e.g. Talreja [118]). Two remarks can be made. Firstly, with cohesive cracks, the role of the strength parameter is less important, since crack propagation is driven primarily by the fracture toughness. Secondly, concerning crack initiation, which is still stress driven, it is unclear to what extent the theoretical relations from fracture mechanics are valid for initiation of cohesive cracks. In contrast with the ply discount method, the stress driven initiation of cracks ought not be related to the energy driven propagation of cracks in fracture mechanics. Nevertheless, as long as only one layer of elements per ply is used, a correction for the in situ effect is appropriate. Therefore the strength parameters are corrected throughout this chapter with the relations proposed by Camanho et al. [14], with the remark that the theoretical underpinning of these relations is not completely consistent with the chosen approach. Shear nonlinearity is neglected in evaluating the in situ parameters.

![Figure 5.1](image-url) Geometry and boundary conditions for notched plate analysis, using symmetry in both in-plane directions.

**Failure mechanism** A material parameter that is not given by Spearing and Beaumont is the fracture energy related to fiber failure. However, this parameter is of high importance for the failure load. Spearing and Beaumont [115] report a far field failure stress of 426 MPa. In the computational results, the maximum load reaches the reported value for $G_{f,c} = 50 \text{ N/mm}$. Therefore, in the following study of this example, this value will be used. Notably, due to the symmetry assumption near the plane of failure the effective value of the fracture energy for fiber failure is two times the input value. The fitting value of approximately 100 N/mm is in the range of values measured for carbon/epoxy by Pinho et al. [99].

In Figure 5.2 the deformation from a post peak time step is visualized. Deformations are magnified with a factor 5. In the top ply (90°), shear nonlinearity is indicated, and in the bottom ply (0°) the fiber damage. In both plies, mesh-independent matrix cracks can be observed, in the top ply as a distributed crack pattern in which
5.1 Notched plate

Figure 5.2 Deformed mesh of both plies with fiber damage $\omega_f$ in the $0^\circ$-ply and shear damage $\omega_{12}$ in the $90^\circ$-ply.

the left most is opening in normal direction and in the bottom ply as a single split with a shear displacement jump.

Damage evolution Figure 5.3 shows the split length (i.e. the length of the discontinuity in the bottom ply which originates from the notch tip in Figure 5.2) as a function of the applied load, where $\sigma_\infty$ is the applied load averaged over the cross section. The evolution of the length of the traction free matrix crack in the $0^\circ$-ply is compared with experimental observations by Spearing and Beaumont [115] and simulation results by Wisnom and Chang [136]. Our results are very close to the latter. The agreement with experimental data is also reasonably well, although the last two experimental data points indicate that the crack propagation is retarded at this stage, which has not been reproduced. Possibly, this retardation is caused by an increase in the fracture energy due to crack bridging with growing crack length, which was not accounted for in the analysis. The cohesive zone is also visualized, as

Figure 5.3 Split length as a function of applied load.
the difference between the complete length of the discontinuity in the displacement field and the length of the traction free crack. The cohesive zone can be observed to be approximately constant at 2.5 mm during crack propagation.

In Figure 5.4(a), the matrix cracking and delamination short before the peak load is visualized. A line is added which indicates the angle of the delamination front with the split in the 0°-ply of 3.5° as reported by Spearing et al. [116]. The agreement with this observation is very well.

![Figure 5.4 Delamination pattern with and without distributed matrix cracking; dotted lines indicate the experimentally observed angle of the delamination front [116]; $\sigma_\infty \approx 410$ MPa.](image)

**Transverse cracking** Extensive transverse cracking can be observed in the computational results. However, in each ply only one matrix crack is opening significantly and the amount of energy dissipated in the matrix cracks is small compared to the energy dissipation due to shear nonlinearity, delamination and fiber failure. Therefore, it is safe to limit the number of cracks in the analysis. Indeed, when the number of matrix cracks per ply is limited to one, this has a very limited effect on the global response. A small increase in the maximum far field average stress value (from 426 to 433 MPa) is observed. The predicted delamination profile is strongly similar in both cases, as can be seen in Figure 5.4.

**Mesh-refinement** The fact that the secondary matrix cracks are not very significant has been used to simplify the following analysis. The number of matrix cracks was limited in all the following analyses, because this allows for use of a coarser mesh in the region without delamination and reduces the number of additional iterations that have to be carried out when cracks propagate. The reduced problem without distributed matrix cracking is subjected to a mesh refinement study. Figure 5.5(a) shows the maximum load level for five different meshes, with uniform refinement in the area where damage occurs. It can be observed that the peak load level is ap-
proximately constant for sufficient mesh refinement. The post-peak response is also independent of the element size (see Figure 5.5(b)).

**Influence of individual models** The analysis is repeated three more times, subsequently turning off shear nonlinearity, delamination damage, and fiber failure. Without shear nonlinearity, delamination is more extensive and a significantly different angle in the delamination front is observed, see Figure 5.6. This is in agreement with earlier computational results by Wisnom and Chang [136]. The obtained load displacement curves are shown in Figure 5.7. The positive influence of delamination on the strength of the specimen can be observed clearly: the maximum load level drops from 433 to 281 MPa when delamination is not allowed. Subcritical delamination reduces the stress concentration at the notch tip and therefore delays the onset of fiber failure.

The increase in delamination when shear nonlinearity is not included does not lead to a strong increase in the maximum load level: the predicted maximum without

**Figure 5.6** Delamination and matrix cracking without shear nonlinearity, $\sigma_{\infty} \approx 410$ MPa, cf. Figure 5.4(b).
Chapter 5 Validation

shear nonlinearity is 439 MPa, which is an increase of less than 2%. Apparently, the shear nonlinearity also reduces the stress concentration with plastic deformations, which in this case cancels the influence of the fact that shear nonlinearity delays delamination. However, this cannot be taken as evidence that it is safe to neglect shear nonlinearity in all cases. The influence of shear nonlinearity on the subcritical damage and the influence of subcritical damage on the load bearing capacity together stress the importance of including shear nonlinearity in failure analysis of composites.

**Thickness effect** Next, the influence of ply thickness on the failure mechanism is investigated by changing the ply thickness from 0.125 mm to 0.5 mm. In Figure 5.8(a) it is shown that changing the ply thickness has a significant influence on the global response. With thick plies, failure occurs in two steps. Delamination propagates more rapidly and the load drops for a first time when the delaminated area reaches the opposite boundary. After that, the delamination propagates rapidly from the plane

![Diagram](image_url)

**Figure 5.7** Influence on global response of disregarding individual failure processes.

![Diagram](image_url)

**Figure 5.8** Influence of ply thickness on response; the dotted line in (b) indicates the experimentally observed angle of the delamination front with $t = 0.5$ mm [116].
of symmetry towards the loaded boundary. When the delamination almost extends over the complete specimen, the load increases again. What remains is an unnotched 0° ligament. The second maximum in the load is reached when this ligament fails. It must be mentioned, however, that for the second maximum, neglecting statistical effects is not realistic. The statistical size effect that exists for the unnotched strength (see e.g. Wisnom [135]) is not included in the current framework.

The ply thickness also influences the shape of the delamination profile. Spearing et al. [116] report an increase in the angle between delamination front and load direction for increasing ply thickness. This trend is reproduced in the computational results, as can be seen when comparing the thick ply results in Figure 5.8(b) with the thin ply results in Figure 5.4(b). However, the angle in the predicted delamination profile is larger than the observed 7°.

Influence of residual stress

Up to this point, residual stresses due to the fabrication process have been neglected. The analysis is repeated with two different values for the temperature drop: \( \Delta T = -50^\circ C \) and \( \Delta T = -100^\circ C \). The influence of the residual stress on the maximum load level is shown in Figure 5.9. The maximum load increases with increasing magnitude of the temperature drop. This can be explained by the fact that the residual stresses promote the delamination because the elastic energy related to the thermal stress is released as delamination drives. And, as observed before, delamination causes an increase in the failure load.

The thick ply analysis is also repeated with residual stresses. In this case, a significant influence is obtained with regard to the load level at which the first load drop is observed. Here, the acceleration of delamination causes a decrease in the peak load level. The load level corresponding with the second peak, however, is independent of the initial temperature drop. This is because after delamination residual stresses have vanished and the remaining fiber ligament that is loaded up to failure is exactly

\[ \text{Figure 5.9 Influence of residual stress on peak load level, for the thick ply analysis, there are two peaks in each analysis: the first related to delamination and the second to fiber failure (cf. Figure 5.8(a)).} \]
equal in all cases. The residual stress did not have a visible influence on the angle of the delamination front.

**Concluding remarks**  The sequence of failure events that has been observed in experiments is reproduced in the presented simulations. The influence of ply thickness on the delamination profile could also be captured. It has been shown that, for this example, distributed transverse cracking does not influence the global behavior, only the primary matrix cracks that initiate at the notch tip are relevant. The influence of residual stress due to the curing process on the load level at which failure occurs can be either positive, negative or negligible, depending on the type of failure.

Shear nonlinearity and residual stress due to the curing process accelerate delamination, which in turn delays the onset of fiber failure. It is exactly this kind of interaction between different processes that complicates failure prediction in laminates. The presented framework is able to capture the different processes and their interaction realistically.

The comparison with reported crack patterns validates the model for matrix cracking, shear nonlinearity and delamination. The model for fiber failure is not validated with the presented analysis, but it is demonstrated that the failure process can be captured with the proposed model.

### 5.2 Open hole tension

A large number of failure experiments have been performed on open hole laminates by Green et al. [29]. Size effects in laminate failure were studied with series of quasi-isotropic specimens involving different types of scaling. In-plane scaling was analyzed as well as two types of thickness scaling: ply-level scaling $[45_{m}/90_{m}/-45_{m}/0_{m}]_{s}$ with $m \in [1, 2, 4, 8]$, and sublaminate-level scaling $[45/90/-45/0]_{n}s$ with $n \in [1, 2, 4, 8]$. The ply-level scaled specimens were fabricated by blocking multiple plies with the same fiber orientation together, thus increasing the effective ply thickness. Numerically, each ply block can be represented as a single ply because delamination is only to be expected at interfaces between two plies with different fiber orientation.

**Table 5.2** Material parameters used in open hole and compact tension analysis; for shear nonlinearity parameters, see Table 5.1.

<table>
<thead>
<tr>
<th>Elasticity</th>
<th>Matrix/Delamination</th>
<th>Fiber failure</th>
<th>Thermal strain</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$</td>
<td>161 GPa</td>
<td>$F_{21}$</td>
<td>$F_{11}$</td>
</tr>
<tr>
<td>$E_2$</td>
<td>11.38 GPa</td>
<td>$F_{22}$</td>
<td>60 (30) MPa</td>
</tr>
<tr>
<td>$G_{12}$</td>
<td>5.17 GPa</td>
<td>$F_{12}$</td>
<td>90 (45) MPa</td>
</tr>
<tr>
<td>$G_{11}$</td>
<td>0.32</td>
<td>$G_{f,c,m}$</td>
<td>0.2 (1) N/mm</td>
</tr>
<tr>
<td>$\nu_{21}$</td>
<td>0.4</td>
<td>$G_{c,m}$</td>
<td>1 N/mm</td>
</tr>
<tr>
<td>$\nu_{23}$</td>
<td>0.4</td>
<td>$\eta$</td>
<td>1 N/mm</td>
</tr>
</tbody>
</table>
The material properties of the individual layers of IM7/8552 carbon/epoxy are taken from Jiang et al. [50], except for those related to shear nonlinearity, which are the same as in Section 5.1. Although much effort is paid to build a robust and efficient framework, two material parameters have been adapted in order to secure robustness for feasible element sizes. For the interface elements, the strength is reduced with a factor 2 as suggested by Turon et al. [124] and examined by Harper and Hallett [37]. Furthermore, for the matrix cracks, the fracture energy related to mode I failure is increased to the value given for mode II failure, viz. from 0.2 to 1.0 N/mm. These parameters are not without influence on the global response. The decrease in interface strength will reduce the peak load level, while the increase in matrix fracture energy will tend to increase it. All material parameters are summarized in Table 5.2. The influence of these changes will be commented upon in the discussion of the results further on in this section.

The value for the ply strength in fiber direction $F_{1t}$ is not uniquely defined, because the strength in unidirectional tests depends on the size of the test specimen due to the importance of the statistical strength distribution [137]. The size of the loaded volume influences the moment of onset of fiber failure. In the analyzed cases, however, with a non-uniform stress distribution and subcritical damage, the loaded volume is variable. The value of 3131 MPa is related to a loaded volume of $1 \text{ mm}^3$. The spacing between the matrix cracks is set equal to 1.0 mm.

The geometry is shown in Figure 5.10. The dimensions correspond with the smallest specimens as tested by Green et al. [29] which is the only in-plane size considered here. In a square region around the hole, the irregular mesh has a uniform density with typical length of the element side of 0.2 mm. In the fine mesh region, matrix cracking and delamination is allowed. Outside the region the mesh is coarser and no cracking is allowed.

**Ply-level scaling** Results for the ply-level scaled specimens are presented in Figure 5.11. Three different values of the maximum load level are shown for each value of
Chapter 5 Validation

$m$, firstly results from plane stress analysis, secondly results from three-dimensional analysis with one layer of solid elements per ply, and thirdly the averaged experimental values. For the cases in which the delamination type failure occurs (see Green et al. [29]), the plotted value corresponds with the maximum load value before the delamination in the [-45/0]-interface reaches the boundary of the fine mesh region. Notably, the delamination type failure mechanism cannot be simulated completely, because it involves delamination over the entire gauge length. But the delamination that is growing from the crack in the $-45^\circ$-ply causes a load drop and the beginning of this process can still be captured well. Therefore, limiting the zone in which delamination is allowed does not influence the peak load values.

The load values are divided by the unnotched cross section, to give a clear visualization of the size effect. Without any size effect, the maximum load would scale linearly with the thickness resulting in a constant maximum far field stress and hence in a horizontal line. It is concluded from Figure 5.11 that the size effect in strength with respect to ply thickness scaling is captured well with the proposed framework, even in two-dimensional analysis.

Not only are the peak load values close to those measured, the failure mechanism in the four different computations also correspond with the observed failure mechanisms. In Figure 5.12 the delamination in the [-45/0]-interface and the fiber damage in the $0^\circ$-ply are shown for a post peak time step for different values of the ply thickness. The results from the analysis with $m = 1$ are typical for the pullout type failure as described by Green et al. [29]: fiber failure in the $0^\circ$-ply and matrix cracking in the others, accommodated by delamination. The results obtained with other values of the ply thickness are typical for the delamination type failure: extensive delamination occurs in the [-45/0]-interface. In the case with double ply thickness, a very small amount of fiber failure is found and in the case with quadruple ply thickness, no fiber failure occurs at all. Results with $m = 8$ are omitted here because they are very similar to those with $m = 4$.

![Figure 5.11](image-url)

**Figure 5.11** Peak load values for ply-level scaling. Comparison between numerical and experimental results for 2D and 3D analyses.
5.2 Open hole tension

![Images of failure modes](image)

(a) $m = 1$: Delamination in $-45/0$-interface
(b) $m = 1$: Fiber failure in $0^\circ$-ply
(c) $m = 2$: Delamination in $-45/0$-interface
(d) $m = 2$: Fiber failure in $0^\circ$-ply
(e) $m = 4$: Delamination in $-45/0$-interface
(f) $m = 4$: Fiber failure in $0^\circ$-ply

Figure 5.12 Typical post peak damage for pullout failure ($m = 1$) and delamination failure ($m = 2, 4$).

A parametric study has been conducted to investigate the influence of adjusting the parameters for robustness. For the case of $m = 2$, a baseline 2D strength of 441 MPa (as per Figure 5.11) was obtained using the values of 1.0 N/mm, and 45 MPa, respectively. Increasing the interface strength up to 90 MPa increased the specimen strength to 503 MPa. After that, reducing $G_{lc}$ to 0.5 N/mm brought it back down to 471 MPa. It can thus be seen that the relative increase in fracture toughness and decrease in interface strength used in the baseline cause effects in opposing
directions and thus the assumptions made to aid convergence of the model solution approximately cancel each other out in these particular cases.

**Matrix crack pattern**  Because this is the first time these tests have been simulated in a framework that can easily deal with many matrix cracks, special attention is paid to the influence of the matrix crack pattern on the results. The series is repeated with a limited number of cracks. In the $\pm 45^\circ$-plies no more than two cracks are allowed, and their location is predefined such that they are almost tangential to the hole. In the $90^\circ$ and $0^\circ$-plies the number of cracks is limited to 2 and 4 respectively, but their exact locations are not specified. This results in a crack pattern similar to that of earlier numerical analyses of these experiments by Jiang et al. [50], where matrix cracks were modeled with pre-inserted interface elements. The computations are done in 2D. In Figure 5.13, results are compared with the previous results with multiple matrix cracks. It can be observed that, in the cases with $m = 2$ and $m = 4$, the influence of the presence of multiple matrix cracks is significant. In these cases, an increase in peak load level is found when the number of cracks is limited.

![Figure 5.13](image_url) Peak load values for ply-level scaling. Comparison between numerical and experimental results, for different matrix crack patterns.

This difference is attributed to the influence of secondary cracks in the $90^\circ$-ply on the delamination near the straight edge of the specimen. In the cases with $m = 2$ and $m = 4$, the maximum load level is associated with load drops that occur when a zone of delamination starts growing from the point where one of the cracks in the $45^\circ$-ply touches the straight edge. In Figure 5.14, the delamination in the $45/90$-interface after the beginning of this load drop is illustrated. It can be observed that in the presence of multiple matrix cracks, the delamination first appears in a small triangular zone that is bounded by two cracks in the neighboring plies next to the long edge of the specimen, while in the case without secondary matrix cracks, delamination grows at once along the whole length of the $45^\circ$-crack. The secondary matrix cracks in the $90^\circ$-ply reduce the load level because they allow for a partial delamination that can be formed more easily.
5.2 Open hole tension

Figure 5.14 Delamination in 45/90-interface after beginning of first major load drop ($m = 4$).

Figure 5.15 Subcritical damage observed in interrupted test specimen ($m = 4$).

In Figure 5.15 C-scan and X-ray images are shown from a test with $m = 4$ that was interrupted shortly before the maximum load level was reached. In the C-scan image, it can be observed that delamination starts primarily near the matrix cracks in the $45^\circ$-ply, as in Figure 5.14, while in the X-ray image, the multiple cracks in all plies are clearly visible. The crack pattern from the simulation for a time step near the maximum load level (Figure 5.15(c)) shows similarity with the X-ray image: individual cracks appear in the $45^\circ$ and $0^\circ$-plies, while matrix cracking is more distributed in the $90^\circ$ and $-45^\circ$-plies. Moreover, the cracks in the $-45^\circ$-ply are located around those in the $45^\circ$ and $0^\circ$-plies. Lesser agreement is found in the length of the $0^\circ$-cracks and the number of those in the $90^\circ$-ply. The latter incongruity may be explained by the fact that all discontinuities are shown in the numerical results, also when they are still cohesive and therefore represent a material degradation that may not yet be visible in an X-ray image.

**Continuum damage model** Furthermore, the series is repeated with a continuum damage model for both fiber failure and matrix cracking. A two-component continuum damage model is used like in Section 2.1, but this time with the crack band
Chapter 5 Validation

method instead of viscous regularization. The same 2D discretization and parameters as above are used, except for the matrix fracture energy $G_{c,m}$, which is increased further for robustness to a value of $3 \text{ N/mm}$. In those cases where failure of the delamination type occurred, the predicted peak load values are far from the experimental values (see Figure 5.16). This is due to the fact that matrix cracks are not necessarily aligned with the fiber. There is a tendency for matrix cracks to grow parallel to the fiber due to the orthotropic elasticity and degradation laws, but this tendency is not strong enough to enforce delamination between neighboring off axis plies.

This is how the limitation of the continuum approach explained in Chapter 2 manifests itself in complete laminate analysis.

In Figure 5.17 the matrix damage is plotted for all plies from a post peak time step for $m = 4$. It can be observed that the matrix crack profile in the $45^\circ$ and $90^\circ$-plies is almost completely matching. Hence, very little delamination is needed between these plies to form a mechanism. Indeed, extensive delamination in the $[-45/0]$-interface, typical of the delamination type failure is not obtained in any of the cases analyzed. Significant delamination does occur between the $90^\circ$ and the $-45^\circ$-ply. This delamination extends towards the boundary of the domain where delamination was allowed before the reported peak load values are reached. Therefore, a completely fair analysis of peak load values predicted with a continuum damage model would require that a larger zone with delamination is allowed. However, the presently obtained results show sufficiently clear that the continuum approach is not suitable for the simulation of failure mechanisms which involve the interaction between matrix cracks and delamination.

Sublaminate-level scaling The thinnest laminate in the series with ply-level scaling is the same as the thinnest in the series with sublaminate-level scaling: $[45/90/-45/0]_{ns}$ with $n = 1$. We repeat the analysis in 2D for $n = 2$, and also for the limit

**Figure 5.16** Peak load values for ply-level scaling. Comparison between numerical and experimental results, for different matrix crack patterns.
5.2 Open hole tension

Figure 5.17 Post-peak matrix damage from continuum damage analysis (ply thickness = 0.5 mm).

Figure 5.18 Through-thickness discretization of [45/90/-45/0]_x and [45/90/-45/0]_∞ laminates.

The peak load values obtained with the proposed model are compared with the experimental values in Figure 5.19. In this case, the size effect is not captured. The experimentally observed decrease in strength for increasing laminate thickness is not reproduced in the simulations. In all simulations the failure is of the pullout type, which does correspond with the experimental observations.
Possibly, statistical strength distribution plays an important role in this size effect. Fiber failure is significant in the pullout type failure and the volume of loaded fibers scales linearly with the thickness. If the statistical strength distribution is the cause for the size effect in sublaminate-level scaling, this would explain why no size effect is present in the numerical results.

Fiber strength Considering the uncertainty of the ply strength in fiber direction, it is interesting to check the influence of varying this parameter on the results. Obviously, the fiber strength does not influence the peak load values in cases where fiber failure is not part of the global failure mechanism. For the cases with pullout failure, however, the parameter is significant, although the failure mechanism also involves delamination. In Figure 5.20 the peak load value is shown for different values of $F_{1t}$. A clear trend is found. The mean experimental value and covariance are shown with dashed lines.

The influence of $F_{1t}$ on the effective laminate strength indicates a drawback of the current framework, because, in fact, this is not a material constant but rather
5.3 Overheight compact tension

The overheight compact tension test has been developed to allow the growth of damage in laminates in a stable manner [52]. A series of overheight compact tension experiments on samples with different laminate designs has been performed by Li et al. [65]. Again, different failure mechanisms were obtained with ply-level scaling and sublamine-level scaling. In this case, the failure mechanisms that involve extensive delamination are computationally prohibitive in our current framework. The in-plane dimensions are larger than for the open hole tests and the element size has to be equally small throughout the delaminated area, which would result in too many degrees of freedom to handle in the implicit solution scheme. The laminates with sublamine-level scaling however, failed without significant delamination. Fiber breakage was observed along the center line, not only in the 0°-ply but also in the ±45°-plies. This failure mechanism is similar to the brittle failure mechanism in the open hole test series [29]. In the compact tension test, however, failure was progressive instead of catastrophic. The failure progressed in small sudden jumps, which were reflected in a series of load drops [65]. Because the same carbon-epoxy material was used as for the open hole experiments, while the failure mechanism was different, it is a valuable validation step to simulate these with the same set of parameters. However, the mechanism without delamination is not found when the

Concluding remarks  With the simulation of open hole experiments, it has been shown that the current framework can be used for accurate simulation of different failure mechanisms in laminates. With the straight matrix cracks and interface elements, the failure mechanisms involving matrix cracking and delamination can be described well and as such modeled accurately. It is confirmed that the same is not possible with a continuum damage model.

In all cases, the failure mechanisms in the computation matched that in the experiment (pullout or delamination). Good quantitative agreement was furthermore obtained for ply-thickness scaling. The correct representation of the failure mechanism allows for the prediction of size effects in failure. However, the size effect with respect to sublamine-level failure has not been reproduced. This is possibly due to the fact that influence of the statistical fiber strength distribution on the onset of fiber failure cannot be captured with the proposed fiber failure description.

Secondary matrix cracks have a small but significant influence on the numerical results. A more important merit of the current approach with the possibility of many matrix cracks, is that the location of the primary matrix cracks is not defined by the user, but rather a result of the computation.
same reduced interface strength parameters are used in the simulation. In the case of the compact tension test, reducing the strength leads to a switch from the fiber failure dominated mechanism to a failure mechanism with significant delamination. The results presented in this section are obtained with the original values for the interface strength. In the absence of large scale delamination this does not endanger numerical stability.

The geometry of the test setup is shown in Figure 5.21. In a band of 8 mm wide reaching to 12 mm beyond the crack tip the mesh is fine with typical element length of 0.14 mm, and only there delamination and matrix cracking is allowed. Outside this region, the plies are completely attached. The sublaminate-level scaling is simplified with periodic boundary conditions as illustrated in Figure 5.18.

**Failure mechanism** The failure mechanism in the simulation is driven by fiber failure in the $\pm 45^\circ$ and $0^\circ$-plies and matrix cracking in the $90^\circ$-ply, as illustrated in Figure 5.22. Minor delamination only occurs in the narrow band with fiber failure ahead of the notch. This is the same failure mechanism as was observed experimentally. Matrix cracks are crucial to form the sawtooth-shaped cracks in the $\pm 45^\circ$-plies, but the energy required to form the matrix cracks is very small in comparison to the fracture energy of the fiber failure. Therefore, the influence of the exact amount and location of the matrix cracks on the global response can be expected to be negligible. From the crack patterns in Figure 5.22, it is concluded that limiting the size of the region with delamination and matrix cracking does not influence the results significantly in this case. Only in the $90^\circ$-ply, the zone with distributed cracking extends up to the boundary of the fine mesh region. The distributed cracking in that ply which is apparently truncated does not interact with the main failure mechanism.
Load-displacement relation  The analysis is performed for different values of the crack spacing parameter. In Figure 5.23, the obtained load-displacement curves are shown. It can be observed that the softening branch is in all cases not smooth, which is due to unsteady propagation of the fiber failure through the irregular mesh. All results fall within a limited band. There is a trend that the load level of the softening branch increases when spacing $\Delta$ is increased, but this trend is not monotonous. Considering the fact that fiber failure is the main dissipative process and that the level of the softening branch in compact tension tests is typically related to the fracture energy, the variation is likely to be connected to the changes in the effective fracture energy of the fiber failure mechanism. Although the fracture energy is input as a material constant, the actual dissipation in the numerical model only matches this value if the assumption of failure in a single band of elements perpendicular to the fiber direction is valid (see Figure 2.14). The input value gives a lower bound, and the accuracy with which this value is approached is determined by the extent to which the mechanism is formed efficiently. This offers an explanation for the observed trend, because with larger spacing, the chance that an optimal mechanism can be formed is reduced. In Figure 5.24, where the fiber failure in the $0^\circ$-ply is visualized for $\Delta = 0.9$ mm, this can be observed in several locations where fiber failure does not form a mechanism in a single band of elements.
Figure 5.23 Load displacement relations for overheight compact tension test: $[45/90/-45/0]_{2s}$ simulations with different values for crack spacing and $[45/90/-45/0]_{2s}$ experiments.

Figure 5.24 Fiber damage and matrix cracking in $0^\circ$-ply in analysis with crack spacing 0.9 mm.

Load-displacement curves from the experiments are also shown in Figure 5.23. The maximum load in the simulations corresponds well with the load level at which the first significant load drop occurred in the tests. However, in the experimental curves, recovery of the load after load drops is visible to an extent that does not occur in the simulations. In two of the five tests, this eventually led to a maximum load that is considerably higher than the values in the simulations.

Alternate approaches Like with the open hole tests, the analysis is repeated with a continuum damage model. The plies are fully attached to each other, so that no delamination is allowed. Notably, this much simpler approach gives results that are strongly similar to those obtained before. The load-displacement curve lies within the band with curves from the more advanced analyses, see Figure 5.25.

The results are also compared with the computational analysis of an idealized system. The quasi-isotropic laminate is substituted with an isotropic material and the crack is modeled as a straight cohesive crack on the center line. This analysis can
be understood as a macroscale analysis, because through-thickness homogenization is performed prior to the analysis. With two different assumptions on the crack orientation in the \(\pm 45^\circ\)-plies, two different values for the equivalent fracture energy \(\tilde{G}_c\) are obtained.

\[
\begin{align*}
\tilde{G}_c &= 78.5 \\
\tilde{G}_c &= 97.5
\end{align*}
\]

**Figure 5.23** Load displacement curves from Figure 5.23 in comparison with simplified models: lumped continuum damage and equivalent isotropic (with two different values for the equivalent fracture energy).

Notably, the softening branches related to the macroscale analyses are much steeper than those from the other simulations and the experiments. The effective fracture energy increases during the simulations as well as during the experiments, although the increase is eventually much larger in the tests. The increase during the simulations is attributed to crack bridging, where the sawtooth crack is not perfect. The increase in the experiments is probably also due to crack bridging (see Pinho et al. [99]). The increase in fracture energy is caused by a deviation from the model assumptions (namely that fiber failure should localize in a single row of elements). That this coincides with reality deviating from the model assumptions (namely that the fracture energy for fiber failure is a ply constant) is not to be counted in favor of the model reliability.

**Fiber strength** Interestingly, the same influence of \(F_{1t}\) is not present in the compact tension test. Reducing the strength from 3131 MPa to 2800 MPa does not give any clear influence on the results, as can be observed in Figure 5.26. The gray patch indicates the results obtained with \(F_{1t} = 3131\) MPa, the colored lines are obtained with \(F_{1t} = 2800\) MPa. The results fall within the same band. Although fiber failure is the dominant process in this failure mechanism, the ply strength in fiber direction is not the most important parameter. This is not completely surprising since the compact tension test is typically controlled by the fracture energy. Nevertheless, it is worth noting that even when fiber failure is dominating the response, the size effect related to statistical fiber strength distribution is not necessarily important.
Concluding remarks  After the delamination type and pullout type failure mechanisms in the open hole tests, in this section another failure mechanism has been simulated. The overheight compact tension test with sublaminate-level scaling exhibits a failure mechanism with crack growth along the center line of the specimen. This failure mechanism involves fiber failure in the $0^\circ$ and $\pm 45^\circ$-plies. This experimentally observed failure mechanism has been retrieved in the simulations. Notably, in this case without significant delamination, the continuum approach gives similar results, even when the whole laminate is modeled with a single layer of elements.

In either case, however, the numerical results do not match theoretical curves for a smooth straight crack on the center line with constant fracture energy. Although constant fracture energy is assumed in the model formulation, the effective toughness is increasing during crack propagation. This mismatch between model assumptions and model results is due to a deviation from the assumption that fiber failure will always localize in a single band of elements. Fiber failure does not always form a perfect mechanism, which introduces crack bridging in the solution. This is worsened by the fact that matrix failure is restricted by the minimum crack spacing. Nevertheless, the influence of the actual value of the spacing on the results is small.

The experimental results also display an increase in effective fracture energy, but in that case it is accompanied by a series of load drops. These load drops, which are associated with brittle crack growth over a finite length, are not reproduced. How to understand these load drops and how to model them is a challenge for the further development of computational models for composite laminate failure.
Chapter 6 Conclusions and discussion

A numerical framework for the modeling of failure in laminates has been developed and tested. Matrix cracks are modeled as mesh-independent discontinuities in the displacement field with the phantom node method, delamination is modeled with interface elements, and fiber failure and shear nonlinearity with continuum damage models. The constitutive models are embedded in an incrementally iterative solution strategy with arclength method and adaptive time stepping. With the proposed framework a new step has been made towards reliable predictive simulation of laminate failure.

New developments

In this work the following contributions have been made to the collection of existing techniques for the computational modeling of laminate failure:

1. Two different continuum models for failure in orthotropic materials with rate dependent regularization have been developed, one based on plasticity, and the other based on continuum damage.
2. The idea to model matrix cracks as straight discontinuities at arbitrary locations with partition of unity based methods has been introduced.
3. Two initially rigid cohesive laws have been developed for matrix cracking in which the singularity for zero opening and zero damage is removed. In both cases the same phenomenological relation between fracture energy and mode ratio is assumed.
4. Van Paepegem’s model for shear nonlinearity has been improved to make it independent of the time step size.
5. A model for fiber failure has been developed for use in combination with a discontinuous description of matrix cracks. The continuum model is regularized with the crack band method.
6. The linearization of Turon’s cohesive law for delamination has been made fully consistent.
7. The concept of a predefined minimum spacing between two matrix cracks in the same ply is introduced.
8. The dissipation-based arclength method has been extended for applications with plasticity, thermal strain and damage.
9. An adaptive strategy with two types of increment and a variable increment size has been implemented, which avoids premature termination of the simulation.

Conclusions

The reliability and accuracy of the different approaches and components have been tested in several numerical examples. The main conclusions from the analyses are:

1. The continuum approach is not appropriate for the modeling of matrix cracks in laminates. The straight orientation of the cracks that is enforced by the microstructure is not ensured in a homogenized model.

2. Straight matrix cracks can be modeled at arbitrary locations in the mesh with partition of unity based methods. Because the crack growth direction is related to the microstructure rather than to the direction of maximum principal stress, a mixed mode cohesive law is needed. For the two cohesive laws that have been introduced the actual energy dissipation is an accurate representation of the prescribed phenomenological function of the mode ratio.

3. The interaction between matrix cracks and delamination is captured accurately when the phantom node method is used for matrix cracks and interface elements are used for delamination. It is for global accuracy not necessary to update the kinematics of an interface element when the elements representing the plies they connect are cracking. This is particularly the case when a nodal integration scheme is used for the interface elements.

4. The interaction between matrix cracks and fiber failure can be described well with a discrete representation of matrix cracks and a continuum damage model for fiber failure when the continuum damage model is orthotropic in its driving force but isotropic in its stiffness reduction.

5. Laminate analysis with discrete matrix cracks that may initiate at arbitrary locations requires that the number of matrix cracks is limited with a minimum spacing. As long as this spacing is chosen sufficiently small to capture the delamination pattern, the precise value of the spacing does not have a significant influence on the global response.

6. Apart from the actual failure processes, other phenomena in laminate mechanics such as matrix nonlinearity and the presence of residual stress due to curing must be taken into account for realistic simulation of complex failure mechanisms. These may influence the rate at which the different failure processes develop and, as a consequence, the type of failure that is critical and the strength of the laminate.

7. The size effect in the tensile ply strength in fiber direction, can be relevant for the modeling of failure of a complete laminate. For some, but not all, failure
mechanisms, the ply strength in fiber direction is important for the laminate strength. The proposed model is not predictive in these cases (e.g. the notched plate and the open hole test with pullout-type failure).

8. Mesh-size independence of all components is ensured. Therefore the same holds for the framework as a whole.

9. For tensile loading on laminates, the failure mechanism can be described well in a plane stress approach where the through thickness variation is represented by interconnecting individually discretized layers with interface elements. The loss of accuracy for neglecting out of plane deformations is small in the considered cases, although there is some uncertainty in the right choice for the elastic interface stiffness.

10. The proposed model allows for realistic modeling of laminate failure. Different failure mechanisms can be described and the appropriate one is ‘chosen’ automatically because the different processes are incorporated realistically.

**Future perspective**

The work in this thesis is limited to static in-plane tensile load cases. It is recommended that the current approach is extended to cover a broader range. Firstly, extension of the framework is possible to dynamics, in which case the solution procedure will have to be different from that presented in Chapter 4. Secondly, to out-of-plane loading. This will require the use of improved elements for three-dimensional analysis, such as the solid-like shell, for which the phantom node method for matrix cracking will have to be adapted. Thirdly, to compressive load cases, with a representation of fiber kinking and of matrix cracks that are inclined instead of vertical.

In the testing of the proposed framework, several issues have been encountered that are of interest for future developments. Most pressing is the statistical size effect for fiber failure. The absence of a representation of the statistical strength distribution of the fiber, disqualifies the framework for simple uniaxial tests on unidirectional specimens and also for some full laminate cases. The strength that is found in such tests depends on the size of the specimen, where in the current model this strength is an input parameter. This cannot easily be solved. The failure mechanism is formed by individual fibers breakages at random locations, which eventually join up with extensive matrix failure to form a failure mechanism. It is not even clear how to formulate a proper kinematical representation of this phenomenon.

Furthermore, regularization in the fiber failure model with the crack band method is not perfect. Limited mesh dependency remains present when the failure progresses through an irregular mesh. Mesh size dependence is solved, but the alignment of the mesh still has some influence on the results.

A serious restriction of the current approach, is that only small specimens can
be analyzed. The cohesive zone must always be discretized with several elements, lest spurious oscillations occur. This has particularly strong consequences for the modeling of delamination, because delamination may extend over large areas. The elements have to be small throughout those areas because the cohesive zone passes everywhere, which draws heavily on the computation time. Adaptive remeshing or techniques that allow for containing the cohesive zone in large elements are possible directions for further research. Multiscale and domain decomposition techniques with automatic refinement wherever that is needed are also potentially useful, as an extension of the fine scale/coarse scale approach in the validation examples in this thesis.

Besides, the applicability of the method would benefit from it if a technique were developed for modeling of the laminate as a whole with a single layer of elements that can still deal with delamination at arbitrary locations. Partition of unity based formulations can be used for the kinematics, but for the initiation and propagation of delamination it is yet to be resolved how the interface tractions can be retrieved accurately without through thickness discretization.

Another open issue is how the in situ effect for matrix cracking can be included best in progressive failure analysis. It has been remarked in this thesis that the models that exist to capture the apparent increase in strength for constrained plies are not compatible with the current cohesive approach. But this observation has not led to a conclusion on what are the most appropriate strength parameters.

Notwithstanding these difficulties that still exist, the development of numerical models for failure to which this work contributes may eventually lead to reliable engineering tools for the prediction of laminate failure. Such tools are not yet available, but the work in this thesis offers a sketch of what they should contain. Potentially, this will lead to a more efficient and flexible design process of composite materials and structures.
References


References


Publications

The greater part of the content of this thesis has been published in scientific publications. Earliest efforts on continuum models that did not make it to the thesis can be found in a chapter in the book *Mechanical Response of Composites*, edited by Camanho et al. [76]. A paper in the *Journal of Composite Materials* [77] has been written to illustrate the limitation of continuum models, as can be found in this thesis in Section 2.1. The idea to use the phantom node method for the matrix cracks (Sec. 2.2) has been published in the *International Journal of Fracture* [78] with emphasis on the bulk constrained cohesive law in Sec. 2.3. The results from the first two papers have been concatenated in a chapter of the book *Advanced Computational Methods in Science and Engineering* edited by Koren and Vuik [79].

The extension to laminate analysis (Ch. 3) has been presented in *Engineering Fracture Mechanics* [80]. Next, the fiber failure and shear nonlinearity models (Secs. 2.5 and 2.6) have been added in a paper in *Composite Science and Technology* [75] including the first validation example (Sec. 5.1). A paper with more extensive validation (Secs. 5.2 and 5.3) has been submitted for publication in the *Journal of Composite Materials* in collaboration with the University of Bristol where the reference experiments have been performed [81]. That last paper also contains a description of the shifted cohesive law introduced in Section 2.4.
Propositions

1. It is hard to break a laminate, even computationally.

2. Continuum models are not suitable for the simulation of splitting of long-fiber materials.

3. Mesolevel failure analysis of composite laminates requires that a minimum crack spacing is enforced between discrete matrix cracks.

4. Mesolevel failure analysis of composite laminates is either performed on a very small specimen or on a very large cluster machine.

5. It is much easier to formulate a numerical model of which you are convinced that it will work, than to implement one of which you can show that it does work. “Don’t think, but look.” (Ludwig Wittgenstein, *Philosophical Investigations*).

6. A numerical example is worth a thousand equations.

7. The researcher’s capacity to argue why his model may be flawed is initially lost at the sight of presentable results.

8. It seems attractive to write cautiously about what seems to be the case, but it is better to present one’s convictions boldly as being the case. “Of course his view must be the right one, or it is not his view.” (G.K. Chesterton, *Orthodoxy*).

9. That there would be a strict separation between objective facts and personal values is not an objective fact.

10. Journalism that is motivated by being critical gives a distorted impression of reality just as state propaganda does, albeit in opposite direction.

These propositions are considered opposable and defendable and as such have been approved by the supervisor, Prof.dr.ir. L.J. Sluys.
Stellingen

1 Het is moeilijk om een laminaat kapot te krijgen, zelfs in een berekening.

2 Continuum modellen zijn niet geschikt voor het simuleren van het splijten van materialen met lange vezels.

3 Mesoschaal bezwijkenanalyse van laminaten vereist dat een minimale scheurafstand wordt ingesteld tussen discrete matrix-scheuren.

4 Mesoschaal bezwijkenanalyse van laminaten gebeurt op een heel klein proefstuk of op een heel groot rekencluster.

5 Het is een stuk makkelijker een model te formuleren waarvan je overtuigd bent dat het zal werken, dan er één te implementeren waarvan je kunt laten zien dat het echt werkt.
   “Denk niet, maar kijk.” (Ludwig Wittgenstein, *Filosofische onderzoekingen*)

6 Een rekenvoorbeeld zegt meer dan duizend vergelijkingen.

7 De kwaliteit van de onderzoeker om te beredeneren waarom zijn model mogelijk niet juist is, gaat in eerste instantie verloren in het zicht van presenteerbare resultaten.

8 Het lijkt aantrekkelijk om voorzichtig te schrijven dat iets het geval *lijkt te zijn*, maar het is beter om overtuigingen stellig te presenteren als *zijn* het geval.
   “Natuurlijk moet zijn visie de juiste zijn, of het is zijn visie niet.” (G.K. Chesterton, *Orthodoxie*)

9 Dat er een strikte scheiding zou zijn tussen objectieve feiten en persoonlijke waarden is geen objectief feit.

10 Journalistiek met als motivatie om kritisch te zijn geeft even goed een vertekend beeld van de werkelijkheid als staatspropaganda, maar dan in tegenovergestelde richting.

Deze stellingen worden opponeerbaar en verdedigbaar geacht en zijn als zodanig goedgekeurd door de promotor, Prof.dr.ir. L.J. Sluys.
Curriculum vitae

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