

# **Enhanced nonlinear analysis of 3D concrete structures**

A thesis submitted to Imperial College London for the degree of  
Doctor of Philosophy (Ph. D.)

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*Creces para ser rey  
y acabas conquistando  
un trocito de acera.*

Ana Merino

*Ponerte a ver el mundo.  
Ir contando sus piezas.  
Y al final descubrir  
que falta una.  
No saber dónde está,  
pero intuir  
que hay una solución,  
que has de dar tú.*

José Corredor-Matheos

**Declaration of Originality**

I hereby confirm that this thesis is my own work. Whenever published or unpublished work of others is used in any way, appropriate references are made.

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## **Abstract**

Although numerical simulation of concrete has a significant background in the framework of simplified one- and two-dimensional elements, a full triaxial description of the structural behaviour of this material is still subject to active research. High fidelity modelling has only been enabled once the required computational capacity achieved an appropriate threshold, and it is precisely of such computational nature that there are diverse drawbacks the material model has to overcome.

For concrete, an existing model combining plasticity and isotropic damage is chosen in this work, and this choice over multi-surface plasticity is duly justified. Additionally, an extension to anisotropic damage is proposed. Focus is set on a series of algorithmic enhancements that significantly increase robustness in stress evaluation, in particular from stress states that pathologically associate to a singular Jacobian matrix and stress-returns that lead towards sensitive areas of the failure surface in principal stress space, where plastic flow is undefined.

Reinforcing steel is modelled as embedded bars inside the corresponding concrete parent elements, with solely axial stiffness. An arbitrary orientation inside the concrete elements is allowed but otherwise the discretised bars share the parent element morphology, order and degrees of freedom, resulting in a perfect bond interaction. An improved and systematic linearising procedure is presented to track the intersections of each bar segment with its embedding parent element, which can be readily applied to any element type and order. This facilitates an accurate calculation of this constituent's contribution to the parent element's stiffness matrix and nodal force vector.

The robustness of the enhanced material model is verified by means of numerical tests, highlighting the convergence ratio, and validation ensues via simulations of established benchmark tests. Finally, some case studies are presented to illustrate the performance of the model at structural level, with insight into various issues of computational nature.

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## NOTATION

All symbols and adopted notation in this work are defined when they first appear. For convenience, the definitions of the most relevant operators and symbols are concisely collected hereafter. It is noted, however, that some symbols may denote more than one quantity; in such cases, the context should provide disambiguation.

### Operators

- Single contraction (e.g.  $\mathbf{A} \bullet \mathbf{b} = A_{ij} b_j$ )
- $\otimes$  Outer product (e.g.  $\mathbf{a} \otimes \mathbf{b} = a_i b_j = (ab)_{ij}$ )
- :
- Double contraction (e.g.  $\mathbf{B} : \mathbf{C} = B_{ijkl} C_{kl}$ )

### Symbols

- $( )^{tr}$  Trial value of the relevant state variable
- $( )^{k,(n+1)}$  Evaluation of relevant state variable at incremental step  $(n+1)$ , iteration  $k$
- $\delta( )$  Perturbation of the relevant entity
- $( )^+, ( )^-$  Limit values of relevant entity from different sides of a discontinuity surface
- $( )_P$  Relevant entity referred to a given point  $P$
- $A^b$  Cross-sectional area of the segment
- $\mathbf{C}$  Elastic compliance tensor
- $\mathbf{D}_e$  Elastic constitutive operator
- $\mathbf{d}_{\xi,P}$  Tangential vector to a bar at a given point  $P$ , in the parent element intrinsic coordinate space
- $\mathbf{d}_P$  Vector of global displacements  $(u, v, w)$  of point  $P$

|                                   |                                                                                                                                                  |
|-----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| $\mathbf{d}_{SE}$                 | Unit vector along a bar axis, comprising its direction cosines $(l_1, m_1, n_1)$                                                                 |
| $E$                               | Young's modulus                                                                                                                                  |
| $e$                               | Eccentricity parameter of the Willam and Warnke function                                                                                         |
| $f_d$                             | Damage loading function                                                                                                                          |
| $\bar{f}_c, \bar{f}_t, \bar{f}_b$ | Compressive, tensile and equibiaxial compressive strength in effective stress space                                                              |
| $\mathbf{F}_{(k)}^b$              | Contribution of bar $b$ to the nodal force vector of parent element $k$                                                                          |
| $f_p$                             | Yield function in effective stress space                                                                                                         |
| $g_d'$                            | Derivative of the damage function with respect to the equivalent strain $\tilde{\epsilon}$                                                       |
| $G_f$                             | Fracture energy (mode I)                                                                                                                         |
| $g_f$                             | Specific fracture energy                                                                                                                         |
| $g_p$                             | Plastic potential                                                                                                                                |
| $H$                               | Generalised hardening modulus                                                                                                                    |
| $h$                               | Characteristic element size parameter / bandwidth estimator                                                                                      |
| $h_{cr}$                          | Critical value of the bandwidth estimator $h$                                                                                                    |
| $I_1$                             | First stress invariant                                                                                                                           |
| $\mathbf{I}$                      | 4 <sup>th</sup> order unit tensor                                                                                                                |
| $ J_R^b $                         | Determinant of the transformation Jacobian between Cartesian coordinates and the intrinsic axial coordinate of the segment pertaining to bar $b$ |
| $J_2$                             | Second deviatoric stress invariant                                                                                                               |
| $\mathbf{J}_{2,\bar{\sigma}}$     | Gradient of $J_2$ in effective stress space                                                                                                      |
| $J_3$                             | Third deviatoric stress invariant                                                                                                                |
| $\mathbf{Jac}$                    | Jacobian matrix of the residual system of equations                                                                                              |

|                                                   |                                                                                                                                 |
|---------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| $\mathbf{Jac}_0$                                  | Evaluation of the Jacobian matrix at initial trial state                                                                        |
| $\bar{\mathbf{J}}$                                | Inverted transpose of the transformation Jacobian between Cartesian and element intrinsic coordinates of a given parent element |
| $\mathbf{K}$                                      | Stiffness matrix                                                                                                                |
| $\mathbf{K}_{(k)}^b$                              | Contribution of bar $b$ to the stiffness matrix of parent element $k$                                                           |
| $k_p$                                             | Derivative of $\kappa_p$ with respect to the plastic multiplier $\lambda$                                                       |
| $K, G$                                            | Elastic bulk and shear moduli                                                                                                   |
| $L$                                               | Length of a given bar $b$                                                                                                       |
| $L'$                                              | Cumulative length of all tracked embedded segments                                                                              |
| $\mathbf{m}$                                      | Gradient of the plastic potential in effective stress space                                                                     |
| $m_V, m_D$                                        | Volumetric and deviatoric invariants of the flow direction $\mathbf{m}$                                                         |
| $m_0$                                             | Friction parameter                                                                                                              |
| $M$                                               | Number of parent elements considered as feasible embedding candidates                                                           |
| $\mathbf{n}_I, \mathbf{n}_{II}, \mathbf{n}_{III}$ | Eigenvectors of the effective stress tensor at trial and returned states                                                        |
| $\mathbf{n}$                                      | Unit normal to the damage band                                                                                                  |
| $\mathbf{N}$                                      | Vector of shape functions                                                                                                       |
| $N_i$                                             | Shape function associated to node $i$                                                                                           |
| $N_{PE}$                                          | Indicator of the location of an entry point relative to the parent element                                                      |
| $\mathbf{p}$                                      | Polarisation vector                                                                                                             |
| $\mathbf{P}_S, \mathbf{P}_E$                      | Start and end point Cartesian coordinates of a bar                                                                              |
| $\mathbf{P}_{k,1}$                                | Cartesian or intrinsic coordinates of entry point into parent element $k$                                                       |
| $\mathbf{P}_{k,2}$                                | Cartesian or intrinsic coordinates of exit point from parent element $k$                                                        |
| $\mathbf{P}_{k,Lj}^{PE}$                          | Coordinates of the exit point from parent element $k$ after $j$ linearisations                                                  |

|                                      |                                                                                                        |
|--------------------------------------|--------------------------------------------------------------------------------------------------------|
| $\mathbf{P}_{k,Lj}^b$                | Coordinates of the point along bar $b$ resulting from $\Delta\alpha_{\min}$ , after $j$ linearisations |
| $q_h$                                | Normalised plastic hardening variable                                                                  |
| $\mathbf{Q}_{EP}$                    | Elasto-plastic localisation tensor                                                                     |
| $\mathbf{Q}_{EPD}$                   | Elasto-plastic-damage localisation tensor                                                              |
| $r(\cos\theta)$                      | Willam and Warnke function                                                                             |
| $\mathbf{r}$                         | Residual vector of the simultaneous system of equations                                                |
| $r_\sigma, r_\rho, r_f$              | Components of the residual vector $\mathbf{r}$                                                         |
| $\mathbf{ref}$                       | Reference vector containing values of all state variables                                              |
| $\Delta\mathbf{ref}$                 | Iterative (Newton) correction of reference vector $\mathbf{ref}$                                       |
| $R_{CN}$                             | Maximum distance between the element interpolation centroid and a node                                 |
| $R_{PS}$                             | Distance between the element interpolation centroid and $\mathbf{P}_s$                                 |
| $\bar{\mathbf{s}}, \mathbf{s}$       | Effective and nominal deviatoric stress tensor                                                         |
| $s_t$                                | Slope of the complementary tensile cone in effective stress space                                      |
| $s$                                  | Cartesian axial coordinate of an embedded segment                                                      |
| $\mathbf{U}, \mathbf{V}, \mathbf{W}$ | Vectors with global displacements of the parent element nodes                                          |
| $W_{gp}$                             | Weight function associated to a given Gauss point                                                      |
| $\tilde{\mathbf{w}}$                 | Complementary damage tensor                                                                            |
| $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ | Vectors with Cartesian nodal coordinates of a given element                                            |
| $\mathbf{x}_c$                       | Cartesian coordinates of the element interpolation centroid                                            |
| $X, Y, Z$                            | Cartesian coordinates                                                                                  |
| $X^*, Y^*, Z^*$                      | Cartesian coordinates of the intrinsic origin ( $\xi = \eta = \zeta = 0$ )                             |
| $x_s$                                | Softening ductility function                                                                           |

|                                                                                    |                                                                                                               |
|------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------|
| $x_h$                                                                              | Hardening ductility function                                                                                  |
| $\alpha$                                                                           | Damping factor for the line search scheme                                                                     |
| $\Delta\alpha$                                                                     | Length of the linearised embedded segment in Cartesian coordinate space                                       |
| $\Delta\alpha_{\min}$                                                              | Minimum admissible value of the linearised length $\Delta\alpha$                                              |
| $\gamma_{12}, \gamma_{13}, \gamma_{23}$                                            | Engineering shear components of the strain tensor in $(\mathbf{n}_I, \mathbf{n}_{II}, \mathbf{n}_{III})$ base |
| $\delta$                                                                           | Kronecker delta                                                                                               |
| $\delta_{23}, \delta_{12}$                                                         | Auxiliary tensors for the algorithmic stiffness derivation                                                    |
| $\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_e, \boldsymbol{\varepsilon}_p$ | Total, elastic and plastic strain tensor                                                                      |
| $\varepsilon_{e1}^{tr}, \varepsilon_{e2}^{tr}, \varepsilon_{e3}^{tr}$              | Principal values of the trial elastic strain tensor                                                           |
| $\varepsilon_{L,P}^b$                                                              | Axial deformation of a given bar $b$ at a point $P$ along its axis                                            |
| $\dot{\boldsymbol{\varepsilon}}_p$                                                 | Rate of the plastic strain tensor                                                                             |
| $\tilde{\varepsilon}$                                                              | Equivalent strain                                                                                             |
| $\dot{\varepsilon}_{pV}$                                                           | Volumetric part of the plastic strain rate                                                                    |
| $\varepsilon_f$                                                                    | Damage parameter controlling the initial slope of the softening diagram                                       |
| $\boldsymbol{\eta}$                                                                | Derivative of the equivalent strain $\tilde{\varepsilon}$ with respect to the strain tensor                   |
| $\Theta_{EP}$                                                                      | Elasto-plastic algorithmic (tangential) stiffness                                                             |
| $\Theta_{EPD}$                                                                     | Elasto-plastic-damage algorithmic (tangential) stiffness                                                      |
| $\theta$                                                                           | Lode's angle or angle of similarity                                                                           |
| $\theta_P^b$                                                                       | Tangential constitutive operator of bar $b$ at point $P$                                                      |
| $\kappa_p$                                                                         | Plastic internal strain-like variable                                                                         |
| $\kappa_d$                                                                         | Internal strain-like damage-driving variable                                                                  |
| $\dot{\lambda}$                                                                    | Rate of the plastic multiplier                                                                                |

|                                                    |                                                                                                                     |
|----------------------------------------------------|---------------------------------------------------------------------------------------------------------------------|
| $\lambda_d$                                        | Damage multiplier                                                                                                   |
| $\Xi$                                              | Pseudo-elastic stiffness tensor                                                                                     |
| $\xi, \eta, \zeta$                                 | Element intrinsic or natural coordinates                                                                            |
| $\hat{\xi}$                                        | Vector of parent element intrinsic coordinates $(\xi, \eta, \zeta)$                                                 |
| $\bar{\xi}_{j,n}^{(type)}$                         | Outer normal to face $j$ of an element of a given type in intrinsic coordinate space                                |
| $\bar{\rho}$                                       | Effective deviatoric radius                                                                                         |
| $\rho_e^{tr}$                                      | Norm of the deviatoric trial elastic strain tensor                                                                  |
| $\bar{\sigma}, \sigma$                             | Effective and nominal stress tensor                                                                                 |
| $\bar{\sigma}_V$                                   | Effective volumetric stress                                                                                         |
| $\bar{\sigma}_1, \bar{\sigma}_2, \bar{\sigma}_3$   | Principal values of the effective stress tensor (ordered $\bar{\sigma}_1 \geq \bar{\sigma}_2 \geq \bar{\sigma}_3$ ) |
| $\bar{\sigma}_{V,apex}^c, \bar{\sigma}_{V,apex}^t$ | Compressive and tensile volumetric stress apex coordinates                                                          |
| $\sigma_{L,P}^b$                                   | Axial stress at point $P$ of a segment pertaining to bar $b$                                                        |
| $\tau_i$                                           | Crack indicator function at node $i$                                                                                |
| $\omega$                                           | Scalar damage variable                                                                                              |
| $\omega$                                           | 2 <sup>nd</sup> order anisotropic damage tensor                                                                     |

# CHAPTER 1

## Introduction

### 1.1 Background

Concrete, either plain or reinforced, has been used as a construction material over a significant time span, allowing the prediction of its structural behaviour and material response under many common scenarios. At the macro-scale level, it can be assumed to maintain isotropy and homogeneity, as the characteristic size of structural members is usually several orders of magnitude greater than the aggregate size. However, the material description of concrete corresponds in reality to a multi-phasic nature where multiple micro-scale phenomena interact to give rise to complex macro-scale effects on stresses and strains.

Nevertheless, the main features of concrete material response are sufficiently well known and constitute the basis of the underlying principles behind technical codes of design. Their scope, however, evolves alongside the social necessities faced by modern structures and the technological advances that progressively increase the requirements on the material.

Ever since the emergence of computational methods for design, numerical models of progressively higher level of sophistication have been implemented and utilised for various structural applications of concrete. In particular, the Finite Element method of analysis has gained the widest popularity. It involves a number of simplifications over the mathematical model that in turn approximates the observable material phenomena. In essence, the main simplification stems from the fact that it discretises the analytical continuous domain (modelling the real material, which is not a continuum) into finite subdomains in which the relevant field variables evolve following assumed interpolation functions. The efficiency of the method, however, has proven to substantially overcome its approximate character provided the scale of the model is moderate, as otherwise the computational cost in terms of memory and processing demands becomes excessive.

In this regard, a compromise has always been required between the complexity of the applied Finite Elements and the available computational power. Consequently, one- and two-dimensional Finite Elements, though with a greater level of approximation than their full three-dimensional counterpart, have a longer development history and still serve as the principal tools for numerical analysis in current engineering practice. Within this framework, so-called high-fidelity modelling aims for an accurate, though still discrete, representation of the true spatial material response of concrete. This is of particular relevance in cases of unusually great dimensions or in parts of a structure where the spatial arrangement leads to complex three-dimensional stress states, as concrete exhibits a size effect (evolving towards perfect brittleness with size) and the interaction with steel reinforcement is not straightforward to assess.

To this end, combining three-dimensional elements with elements of lower dimension, called mixed-dimensional coupling (Izzuddin and Jikhio, 2016; Mata *et al.*, 2008), offers an interesting balanced alternative, as it allows to assign computational resources according to the fidelity necessities (Figure 1.1).

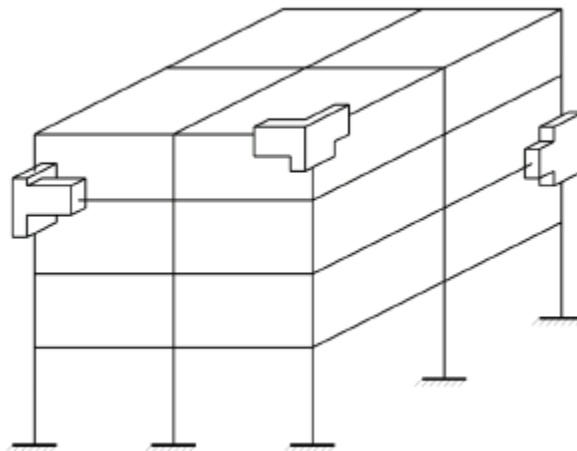


Figure 1.1: Spatial frame with mixed-dimensional coupling (Jikhio, 2012)

For mixed-dimensional coupling analysis to succeed, however, the underlying material model of the three-dimensional concrete elements needs to attain a high level of robustness. Hence, the choice of a suitable material model following the criteria and properties described in this thesis must be weighed with due consideration of accuracy and computational efficiency. Essentially, the proposed triaxial material model algorithm has to balance the demand of high fidelity modelling and still offer a high computational performance.

## 1.2 Scope and objectives

In the frame of finite element analysis, several attempts have been made towards a consistent and generally applicable discrete model of structural elements made of plain or reinforced concrete. These have achieved various levels of success for specific subsets of problem where a simplified one- or two-dimensional approach still leads to fair estimates of the analytical solution. On the other hand, the more complex and general three-dimensional case is still currently an active research field, specifically within the recent stream of high-fidelity modelling alongside mixed-dimensional coupling.

The main sources of nonlinearity when modelling reinforced concrete are of material nature, rather than geometric. Hence, intrinsic properties of concrete, such as inelasticity, anisotropy and heterogeneity, together with its time-dependent behaviour, make it difficult to define three-dimensional constitutive relations. The main empirical phenomenon associated with these material nonlinearities is well established: fracture. However, the reference scale and constitutive modelling of this phenomenon are still the subject of various distinctive approaches, the resulting definitions being also diverse and with different mathematical implications in the formulation depending on the so-called softening potentially entering the stress-strain relations.

Considering the aforementioned context, the main objectives of this thesis are:

1. Rational selection of an appropriate three-dimensional material model of concrete to account for its main sources of material nonlinearity. The selection aims at the model being used as a benchmark for large scale structural simulations, complementing existing one- and two-dimensional elements where high-fidelity should not be necessary. For the constituent concrete, nonlinearity mainly involves fracture and long-term effects. Whilst the former guides the elaborations of the present research, the latter is left outside the scope of work but could be incorporated in the future.
2. Assessment of the key parameters influencing the numerical robustness and performance of the selected concrete material model. Computational cost is one of the drawbacks for full three-dimensional numerical analysis not being widely applied to larger scale projects. Hence, a main aim of this research is to identify the sources of convergence failure or convergence rate decay of the model.

3. Development of enhancements to alleviate or remedy the numerical issues hindering robustness and performance. Numerical methods of analysis, like the Finite Element Method, resort to evaluation of state variables at selected sample points to integrate the rate form of the constitutive equations incremental-iteratively. Therefore, enhancements at sample point level have a significant beneficial effect when solving the global boundary value problem.
4. Development of an efficient algorithm to incorporate the one-dimensional reinforcement bars within the three-dimensional concrete mesh. Locating each bar efficiently and discretising it consistently with the embedding concrete parent elements poses algorithmic challenges that need to be addressed in line with the aforementioned aims of robustness.
5. Investigation of the effects of the applied regularisation technique on the performance of the model. In most cases, the failure modes associated to concrete entail localisation, which in turn leads to potential loss of mesh-objectivity and mesh induced directional bias. Whilst the crack band approach is a remedy for the former, the latter requires further insight.

In this research, and particularly based on objectives 2-4 above, focus is placed on algorithmic development, and it is mainly within this framework where the originality of the work lies. Novel algorithmic enhancements are provided for the two constituents, at material level for concrete and at geometric level for the reinforcement bars. Robustness is shown to improve by means of numerical tests with full convergence ratio, which previous works fail to attain. An approach to reconcile ambiguities in stress evaluation of hydrostatic states is also proposed, and the damage definition is extended to reflect anisotropy.

### **1.3 Outline of thesis**

This thesis comprises seven chapters overall. The current chapter provides a basic background to the main research topic introduced immediately thereafter. The scope of work is described and its objectives are established.

Chapter 2 provides an extensive literature review, specifically oriented towards the phenomenon of fracture. Different working scales are assessed and the choice of macro-scale is justified as the reference scale. Several model formulations of cracking, both discrete and

smearred (in a broad sense) are reviewed. In each case, their main advantages and drawbacks are highlighted and commented upon, leading to the reasoned selection of a combined plastic-damage model formulation on which to base the development elaborated in subsequent chapters.

Following the choice of a material model formulation, Chapter 3 proceeds to describe thoroughly one such model and introduces its algorithmic treatment. The main challenges overcome by the proposed algorithm are elaborated, with focus on Jacobian singularity, along with the suggested techniques for its remedy: system reduction and a line search strategy. An extension of damage to account for anisotropy is proposed and formulated. The enhanced robustness of the model is verified by means of a numerical test, where the displayed convergence rate is significantly improved. Localisation analysis is applied to the model to corroborate its good directional properties, and the regularisation strategy, formally based on the crack band approach, is introduced and justified.

Chapter 4 describes the modelling of the reinforcement. Upon review of the main alternatives, the embedded approach is selected for implementation. Emphasis is made on its algorithmic structure, comprising novel strategies for the discretisation of a steel segment consistently within the embedding concrete mesh. The tracking procedure for successive embedded segments is presented, and it is shown to accommodate without ambiguity any possible configuration with respect to the concrete parent elements. The proposed method of bar discretisation is systematically applied to all the element types considered, including the treatment of the singular pyramid apex. Subsequently, the contributions of an embedded segment to its parent element in terms of stiffness and nodal forces are formulated for the cases of geometrically linear and nonlinear analysis. A single element control test is performed to verify the composite nature of the combined material response.

Following the algorithmic description of both constituents, Chapter 5 provides a series of validation studies in the form of simulations of benchmark testing on laboratory sized specimens. The associated failure modes cover a wide range from the commonly observed failures of structural members, and serve the purpose of validating the algorithmically enhanced material model. Additionally, and throughout the various simulations, specific topics presented in previous chapters are investigated. In particular, the convenience of the damage bandwidth having the character of an external fixed parameter as opposed to an

internal variable resulting from a projection method. Mesh-induced directional bias is evaluated by considering different mesh topologies in the area of damage propagation and the effect on performance of applying localisation analysis to determine the orientation of the damage bands is also assessed. To a lesser extent, computational issues like the potential benefits of hierarchic partitioned modelling are also considered.

Two major case studies of a larger scale are investigated in Chapter 6, whereby in both cases the associated failure mechanisms are not thoroughly treated in the technical literature or current codes of design, and are still active topics of research. In the first case, a very deep beam (representative strip of a slab), cast in the framework of a prediction contest, loaded asymmetrically and meant to fail in shear in the unreinforced span, is simulated resorting to isotropic and anisotropic damage, as well as to static and dynamic analysis. The effect of the assumed material homogeneity on such a voluminous specimen is assessed, and an interpretation in terms of energy balance is suggested to account for the accentuated snap-backs observed in simulations but not in the experiment. The second case study comprises the simulation of reinforced slabs tested to fail in punching shear by either crushing of compressive struts on the column head or within the zone of shear reinforcement. Predictions of strength and slab rotations at failure are compared against experimental observations, as well as the damage pattern along a slab cross section.

Finally, Chapter 7 provides a summary of the main conclusions and achievements of the current research, along with suggestions for future work towards further enhancements of the material modelling of reinforced concrete.

# CHAPTER 2

## Literature review

### 2.1 Introduction

In this chapter, an extensive review on the modelling approaches to fracture is made, inasmuch as it constitutes the main source of nonlinearity in the material response of concrete. The appropriate scale constituting the framework of the reviewed models is first duly justified, in line with the aim at efficient modelling at structural level. Subsequently, the main formulations within the discrete and smeared approach are summarised, extending the sense of the latter to include plasticity and damage. In each case, the main benefits and drawbacks are highlighted, with focus on performance at global level, alteration of the constitutive relations and potential locking.

An overview on regularisation techniques based on the notion of nonlocal continuum ensues, providing the required internal length scale upon loss of well-posedness of the global boundary value problem.

A shortlist of combinations of the individual formulations, conveniently complementing each other, is reviewed in the last section, comparing their properties and assessing their deficiencies. As a result, the final choice of material model for concrete on which to focus subsequent chapters is made.

## 2.2 Reference scales for modelling

Concrete is, by its nature, a highly heterogeneous and anisotropic material. It attains its hardened state upon evolution of several chemical reactions, triggered by the mixture of water, hydraulic binder and aggregates. These reactions actually continue to take place for a long time span, and affect the long-term behaviour of the material as well. The resulting micro-structure is highly irregular, the different constituent phases (silicates and aluminates) and residuals being responsible for different observable characteristics. At this micro-scale, however, it is not possible to describe deformations in a straight-forward manner because of the multi-phasic nature of the material. The amount of information to be processed for a significant volume of material is too vast, which makes this frame impracticable for large-scale structural modelling.

Meso-scale modelling ‘zooms out’ the resolution on the constituents and considers hardened concrete to be tri-phasic, i.e. an irregular distribution of aggregates of various sizes and flaws/voids embedded in a cementitious matrix (where the flaws are usually disregarded and the interface between aggregate and matrix is assumed as an independent phase with its own material properties). Although this scale is still accurate at describing the heterogeneity of concrete, it needs statistical tools to process the randomness in the spatial distribution of constituents, which in turn leads to a random scatter in terms of energy dissipation upon deformation. This combination of statistical and mechanical processes has been formulated in recent years (Grassl and Jirásek, 2010) for the case of material tests under uniaxial conditions, on the basis of lattice and particle models. However, its generalization to triaxial states and the structural testing scale is still the subject of research at present. Since this thesis is aimed at efficient modelling at the structural level, the computational cost of a statistical description does not appear to be acceptable at its current state, and hence meso-scale modelling is also discarded as the frame in which formulations are to be elaborated, although it is recalled in subsequent sections to further illustrate the processes phenomenologically approached in the adopted scale, to be reviewed hereafter.

Finally, macro-scale modelling considers concrete to be a one-phase material, based on the notion of continuum, that is, a material filling every point in the space it occupies, which is very convenient from the mathematical perspective because it naturally allows for the use of continuous tensorial functions as considered in the general theory of elasticity. At this scale,

aggregates and matrix bridges between these are much smaller than any characteristic dimension of a given concrete body, thus they become indistinguishable from each other and only ‘merged’ variables (later to be called effective or nominal, depending on the case) representing the combined average properties of both will enter the formulation. This average character over a great volume of material, with randomly distributed aggregates throughout the matrix, justifies the assumption of the continuum being homogeneous and isotropic at the macro-scale. All material models reviewed in the following sections are formulated within this scale, although some are based on deviations from macro-isotropy.

## 2.3 Fracture

There is a great deal of experimental evidence showing the material nonlinear behaviour of concrete beyond a certain load threshold. At lower scales, it appears as a natural outcome that deformation takes place along with fracture, which is definitely the main source of such nonlinearity, at almost every stage of the loading process. After some initial atomic displacements of viscous-elastic nature, decohesion of the interface between matrix and aggregate starts taking place, thus forming micro-cracks that tend to propagate towards the matrix until these coalesce into macro-cracks, which in turn end up constituting tortuous discontinuities that physically separate the material volume (Lemaitre and Chaboche, 1990). As a reference, Fig. 2.1 shows the basic stages just described for a mixed mode fracture (i.e. opening and in-plane sliding of the crack lips, or mode I and mode II respectively).

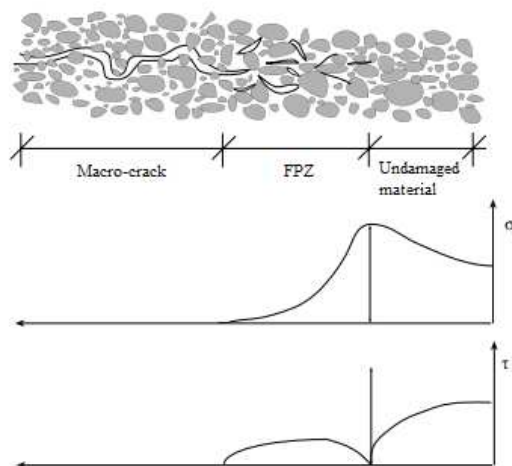


Figure 2.1: Evolution of fracture process zone and stresses under mixed-mode fracture (Gálvez and Cendón, 2002)

Concrete is to be modelled as a continuum with initial Hooke material properties, following the choice of macro-scale, and hence what appear to be cross-effects at this macro-level, like pressure sensitivity of inelastic shear strain and dilatancy (Jirásek and Bazant, 2002) or coupling between deviatoric and hydrostatic states, require the use of *internal variables*, non-directly measurable entities that represent the effect of lower-scale phenomena in the continuum. The different ways in which sets of internal variables are used to translate these effects into a macro-scale continuum formulation defines the philosophy behind the different models to be reviewed in this chapter.

Fig. 2.1 schematically shows an important feature of concrete fracture. Although micro-cracks start propagating throughout the matrix in the fracture process zone (FPZ), there are still undisrupted matrix bridges as well as imbricated aggregates that allow for a progressively decreasing stress transfer. This transition process between a continuous stress distribution and the physically separated and unstressed crack lips is characteristic for concrete and the so-called quasi-brittle materials where the FPZ is not negligible, as opposed to perfectly brittle materials, in which this zone tends to zero and the stress transition tends to a sudden drop, and ductile materials, where the process zone mostly undergoes yielding (Fig. 2.2). In fact, concrete was originally considered a perfectly brittle material and Linear Elastic Fracture Mechanics (LEFM) emerged as the tool to model it. However, LEFM cannot overcome a series of drawbacks, like the high dependence on specimen geometry and size or the inability to describe cracking when no initial macro-crack is present (Planas *et al.*, 2003). This precisely describes the situation in which further nonlinear approaches to fracture had to be developed: they need to have the nature of constitutive assumptions, applicable anywhere within the material and not just ahead of a pre-existing crack tip (Planas *et al.*, 2003).

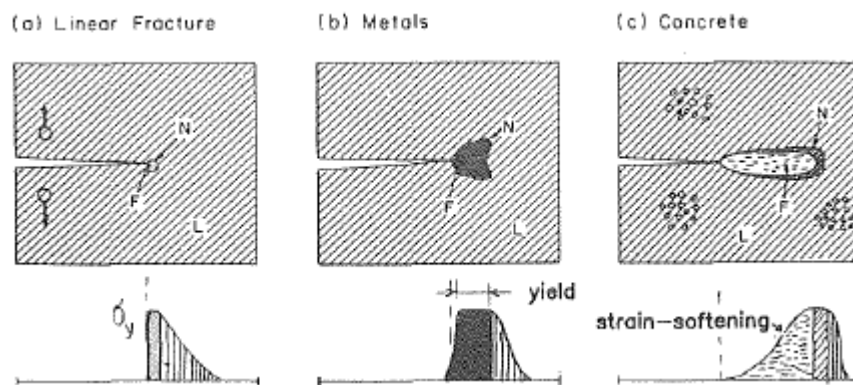


Figure 2.2: Different FPZ for brittle, ductile and quasi-brittle materials (Bazant, 1986)

Generically, constitutive macro-scale models for concrete can be divided in two types:

- Discrete
- Continuum based (smeared)

Discrete models concentrate the decohesion of the FPZ in lines (bands of zero width, for later ease of comparison), discontinuities dividing (not necessarily with a physical separation) portions of continuum where non-fracturing constitutive relations still apply. Continuum based models strictly comply with the chosen macro-scale continuum nature, as decohesion is assumed to take place in finite regions of the material (for simplicity, bands of finite width) and appropriate modifications have to be made in the relations between stress and strain tensors to account for this. Both model types are simplified macro-scale approaches but the difference between these, though formally arbitrary, has important consequences when elaborating formulations, as remarked for the particular models reviewed in the following sections.

Compressive states also imply nonlinear processes involving dislocations and rearrangements at lower scales but these can be captured as in the second fracture model type, i.e. with continuum formulations that alter the stress-strain tensor relations appropriately. In any case, both load responses exhibit a characteristic feature, illustrated in Fig. 2.3 for the case of uniaxial compression.

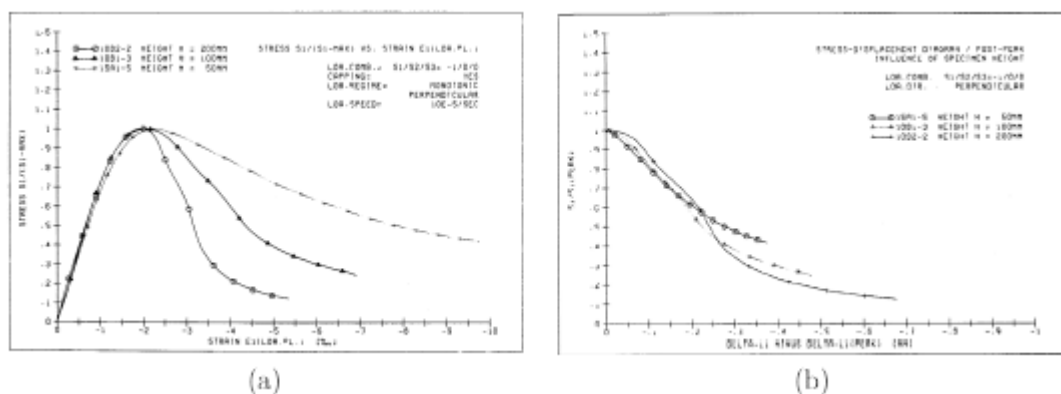


Figure 2.3: Concrete prisms of varying length: nominal stress as function of (a) nominal strain (b) top displacement minus its value at peak (van Mier, 1984)

In the stage prior and up to the peak load, nominal stress curves for different prism sizes fairly coincide, and there is a unique relation with the nominal strain. At peak load, the deformation pattern changes from macroscopically homogeneous deformation to localised

shear bands or cracks. The structure experiences macroscopic strain softening, i.e. the nominal stress decreases with increasing nominal strain (Rolshoven, 2003). In essence, this is the same softening character showed by the curve of cohesive fracture in Fig. 2.1. In the post-peak range, however, there is a clear tendency from ductile to brittle behaviour upon increase of the specimen length. A dimensional analysis of the physical problem using the  $\Pi$ -theorem can be shown to reveal that at post-peak an additional material parameter with dimensions of length is needed (Rolshoven, 2003), hence the uniqueness of the relation of nominal stress with relative displacement. This dependency on a parameter with dimensions of length is called the ‘size effect’ and it can be generalized to two- and three-dimensional cases (Bažant and Planas, 1998). For concrete, the size effect is typically accompanied by localised deformation patterns and reduction of transmitted stresses, and herein lies the need for strain softening curves, to describe localisation with continuum-based type models (Rolshoven, 2003).

### 2.3.1 Discrete crack models

Discrete models for cracking are based on displacement jumps concentrated in bands of zero width. The evolution of such displacements with tractions across the crack following the softening shape as depicted in Fig. 2.1 is the core of the originally called fictitious crack model (Hillerborg *et al.*, 1976), that later evolved to become the cohesive crack model (Planas *et al.*, 1993). According to Planas *et al.* (2003), the three main elements for a material formulation by means of this model are :

- The stress-strain behaviour of the material in the absence of cracks. This may refer back to classical constitutive modelling in terms of general elasticity or further relate to elasto-plasticity.
- An initiation criterion to determine the conditions under which a new cohesive crack will form and which orientation it will have.
- An evolution law for the cohesive crack, relating transferred stresses across the crack to the relative displacements between crack lips.

Regarding the last two points, initially cohesive models were developed for monotonic mode I cases. Consequently, the maximum principal stress was the only stress component involved and the cohesive stress was uniquely a function of the crack opening (Fig. 2.4).

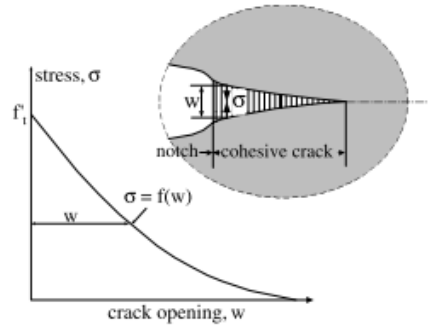


Figure 2.4: General definition of the softening curve: stress-crack opening curve  
(Planas *et al.*, 2003)

The fracture energy (under mode I)  $G_f^I$  is defined as the energy required to create a unit surface of cohesive crack. Assuming it as a material property is arguable though usual, and approximations like neglecting any energy dissipation outside the cohesive crack as well as the absence of triaxial dependency were considered intrinsic limitations of the formulation that called for further generalizations (Planas *et al.*, 2003). Extension of the model for mixed mode loading is an advance in this regard. It is based on a formally similar set of equations as in non-associated plasticity (Section 2.4), although the stress functional is called fracture surface, the scalar equivalent parameter is an inelastic displacement and softening is explicitly defined for cohesion as well (Gálvez and Cendón, 2002) (Fig. 2.5), giving rise to an additional form of fracture energy,  $G_f^{II}$ . The resolution of the resulting nonlinear system of equations follows the same lines of reasoning as in the case of plasticity.

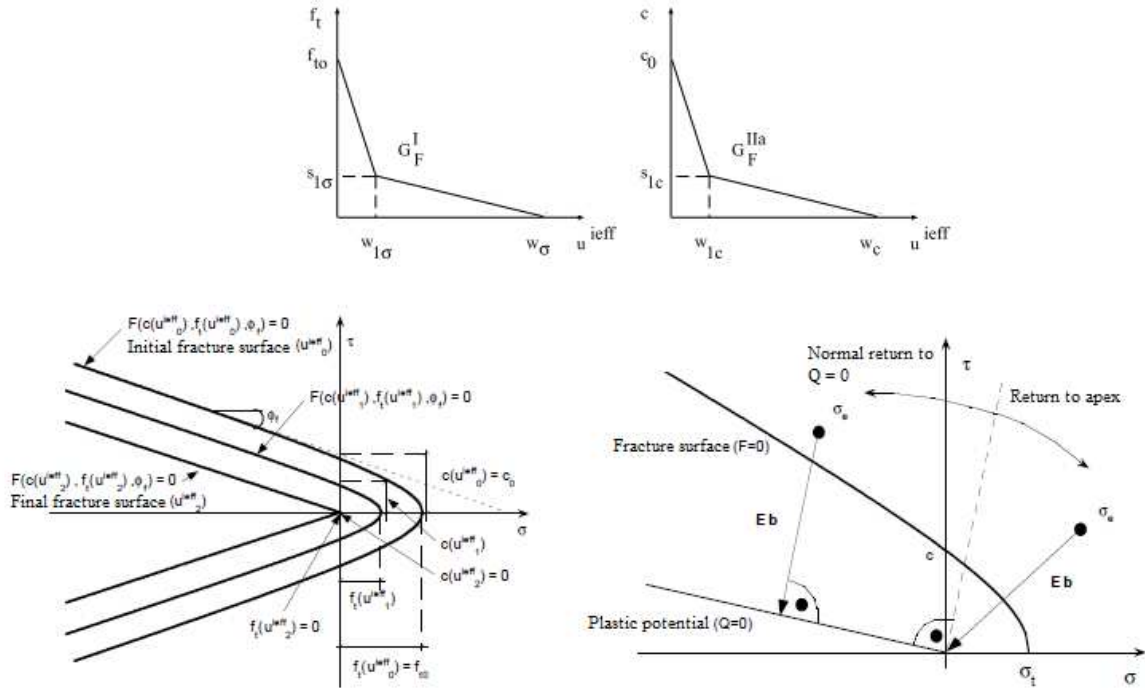


Figure 2.5: (top) Softening curves for modes I and II (left) Evolution of fracture surface (right) Direction of return of inelastic predictor (Gálvez and Cendón, 2002)

The most intuitive way to incorporate a discrete crack in a finite element mesh is by enforcing it to follow the element boundaries, which calls for the use of interface elements. These include the appropriate modes depending on the element dimension and can be either lumped, evaluating tractions and displacements at isolated node-sets, or continuous, smoothing the behaviour along an interpolated field (Rots, 1988) (Fig. 2.6). Although the latter type could be considered to be better, there are numerical problems arising from the very large penalty stiffness necessary to keep initial separations negligible, as it might induce significant flutter in traction profiles (Rots and Blaauwendraad, 1989).

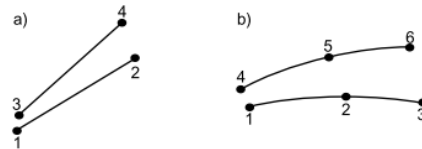


Figure 2.6: Interface elements (a) linear (b) quadratic (Gálvez and Cendón, 2002)

Nonetheless, there are various situations in which it is not possible to know *a priori* what path the cracks will follow and hence a certain mesh-induced crack tortuosity has to be

accepted; alternatively, elaborated re-meshing techniques become necessary to maintain alignment between interfaces and element boundaries (Fig. 2.7).

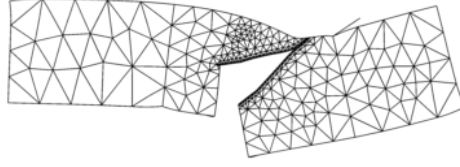


Figure 2.7: Deflected F.E. mesh simulating fracture with adaptive re-meshing  
(Gálvez and Cendón, 2002)

Attempts to generalize the interface discrete approach, decoupling discontinuity orientation from mesh geometry, together with the need to overcome the problem of stress-locking (as addressed in Section 2.3.2), led to the concept of embedded discontinuity (Belytschko *et al.*, 1988; Dvorkin *et al.*, 1990; Ortiz *et al.*, 1987) i.e. a lumped jump of displacement (strong discontinuity) and strain (weak discontinuity) inserted in the interior of a finite element. This discontinuity may have any orientation, normally dictated by the maximum principal stress, and does not imply disruption in the discretized bulk material, which keeps its constitutive law unchanged. The discretised displacement and strain fields are decomposed into a continuous part (bulk) and a discontinuous part (crack) that is collected in additional degrees of freedom:

$$\mathbf{u} = \mathbf{N}\mathbf{d} + \mathbf{N}_c\mathbf{d}_c \quad (2.1)$$

$$\boldsymbol{\varepsilon} = \mathbf{B}\mathbf{d} + \mathbf{G}\mathbf{e} \quad (2.2)$$

where  $\mathbf{d}$ ,  $\mathbf{d}_c$ , and  $\mathbf{e}$  are column matrices containing the nodal degrees of freedom, the additional enhanced displacement modes and the additional enhanced strain modes, respectively. The displacement and strain fields are enriched with  $\mathbf{d}_c$  and  $\mathbf{e}$  via the matrices  $\mathbf{N}_c$  and  $\mathbf{G}$ , supplementing the usual interpolation expressions resulting from the shape function matrix  $\mathbf{N}$  and its derivative  $\mathbf{B}$ . Additionally, the stress field in the discretised problem is approximated as:

$$\boldsymbol{\sigma} = \mathbf{S}\mathbf{s} \quad (2.3)$$

where  $\mathbf{S}$  stands for a matrix interpolating stresses from  $\mathbf{s}$ , a column matrix collecting stress parameters. Subsequently, these unknown field approximations are used to calculate traction separately from the bulk strains and stresses, whereby internal equilibrium is in general

enforced in a weak sense (Jirásek and Zimmermann, 2001), leading to the following set of discretised equilibrium equations derived from the Hu-Washizu variational principle:

$$\int_V \mathbf{B}^T \tilde{\boldsymbol{\sigma}}(\mathbf{B}\mathbf{d} + \mathbf{G}\mathbf{e}) dV = \mathbf{f}_{ext} \quad (2.4)$$

$$\int_V \mathbf{G}^T \tilde{\boldsymbol{\sigma}}(\mathbf{B}\mathbf{d} + \mathbf{G}\mathbf{e}) dV - \int_V \mathbf{G}^T \mathbf{S} dV \mathbf{s} = \mathbf{0} \quad (2.5)$$

$$\int_V \mathbf{S}^T \mathbf{B}_c dV \mathbf{d}_c - \int_V \mathbf{S}^T \mathbf{G} dV \mathbf{e} = \mathbf{0} \quad (2.6)$$

$$\int_V \mathbf{B}_c^T \mathbf{S} dV \mathbf{s} = \mathbf{0} \quad (2.7)$$

where  $\tilde{\boldsymbol{\sigma}}(\boldsymbol{\varepsilon})$  is the stress as computed from the strain field via the constitutive equations. Depending on the approach followed to solve the system (2.4)-(2.7), the stress continuity or displacement/strain discontinuity may not be fully satisfied. A thorough revision and classification of all approaches within a unified framework can be found in (Jirásek, 2000; Jirásek, 2014).

A further method to insert strong discontinuities across finite elements is based on an enhancement of the displacement field and the partition-of-unity method (Babuška and Melenk, 1997). Additional degrees of freedom and enhancing functions (called enhanced basis terms) fulfilling certain requirements are incorporated in conventional finite element formulation (called in this case extended or X-FEM). If the enhanced basis terms are chosen to coincide with the Heaviside function, a displacement field crossed by a single discontinuity, but otherwise continuous, will be exactly described. Thus, the partition-of-unity property of finite element shape functions can be used in a straightforward fashion to incorporate discontinuities in a continuum such that their discontinuous character is preserved (de Borst *et al.*, 2012). Should the discontinuity coincide with an element border, the interface formulation would be retrieved, with the advantage that cohesive surfaces are only placed at onset of decohesion, thereby avoiding the problem of assigning large penalty stiffness values that lead to the traction oscillations noted before (de Borst *et al.*, 2012).

It is important to note the *external* characterization of softening, which is concentrated along bands of zero width that may not necessarily coincide with element boundaries, and that the classic constitutive relations between strain and stress tensors are not altered because the bulk

material is considered to be completely free of fracture. Hence, the additional cohesive relationship between traction and separation does not change the mathematical definition of the problem (as in Fig. 2.3b, where the solution in terms of relative displacement is still unique), i.e. there is no need for internal length scales. The fracture energy, with the noted simplifications, remains insensitive to mesh geometry and the particular softening curve shape, disregarding disquisitions about its material nature, remains of limited relevance. In fact, when the size of a structural component is much larger than the cohesive zone size, the peak load is fully controlled by the fracture energy, irrespective of the softening shape, whereas for not too large specimens and uncracked samples, tensile strength and the initial slope of the softening curve become the controlling parameters because in such cases the peak load occurs at low separation values and therefore strength is fully defined by the initial linear portion of the softening curve (Elices *et al.*, 2002).

If the softening function were to be determined experimentally, there are some drawbacks that call for indirect methods like inverse analysis. The first drawback is related to the material real heterogeneity, leading to unpredictable location and number of cracks occurring. This is also the reason behind the inclusion of material imperfections rather than performing bifurcation analysis (Bažant and Planas, 1998). The second drawback is the tendency to asymmetric modes of fracture (Elices *et al.*, 2002)(Fig. 2.8). However, this asymmetric behaviour under direct tension can also be numerically captured with the use of imperfections (Rots, 1988).

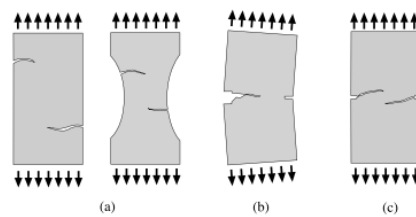


Figure 2.8: (a) Multiple cracking in tensile specimens (b) Rotation of crack faces in pre-cracked specimens (c) Crack overlapping (Elices *et al.*, 2002)

### 2.3.2 Continuum-based smeared crack models

Continuum-based models do not lump discontinuities in surfaces of zero thickness. Instead, they affect the bulk material (i.e. the interior of finite elements upon discretisation) at constitutive level, distributing the nonlinear material responses across finite regions. This

approach allows for preservation of the original element mesh and, depending on the case, of isotropy at macro-scale as well.

The smeared crack concept was originally introduced by Rashid (1968), and its formulation was systematised by Rots (1988). It is based on the constitutive description of a cracked continuum that changes initial macro-scale isotropy to an orthotropic law upon crack formation, with the axes of orthotropy being determined according to a condition of crack initiation (Rots and Blaauwendraad, 1989).

Local strains are decomposed, similarly to displacements in the case of embedded discontinuities, into bulk material strains and crack strains:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_c \quad (2.8)$$

These relate to different constitutive operators, the former being usually taken as the elastic one and the latter being responsible for the inclusion of strain softening in the formulation, that is a gradual decay of nominal stresses with increasing nominal strains through appropriate changes in their constitutive relations, as opposed to a sudden stress drop. This can be formally expressed as:

$$\boldsymbol{\sigma} = \mathbf{D}_e : \boldsymbol{\varepsilon}_e \quad (2.9)$$

$$\mathbf{t}_c = \mathbf{f}_c(\mathbf{e}_c) \quad (2.10)$$

with  $\mathbf{t}_c$  and  $\mathbf{e}_c$  being the traction vector acting on the crack plane and its strain work-conjugate, related by function  $\mathbf{f}_c$  and expressed in the local coordinate system aligned with the crack. An incremental approach is followed for the resolution of stresses. This implies linearization around a reference state and iterative corrective procedures like the general Newton-Raphson scheme.

Depending on the number of cracks allowed per sample point and the changes of orientation, three main smeared crack models can be distinguished, as illustrated in Fig. 2.9:

- Fixed single crack
- Multi-directional crack
- Rotating crack

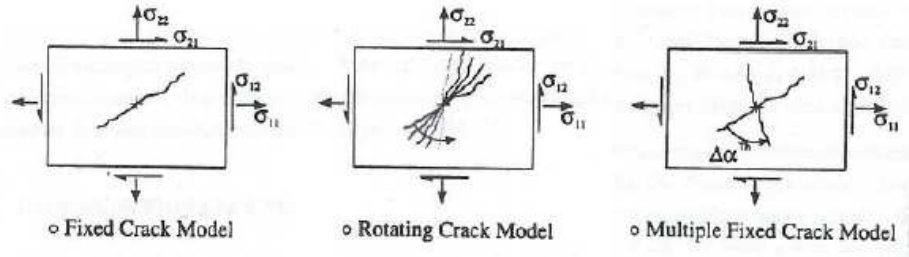


Figure 2.9: Classic smeared crack models (Weihe, 1995)

The fixed single crack model considers a single crack that does not change its orientation, which is convenient for the handling of crack state changes. Indeed, upon an incremental step, a new crack may form, an open crack may close or a closed crack may re-open. The criteria to define these changes are generally expressed in terms of total local strains or stresses. Since the local axes remain unaltered, these quantities are readily available in the form of an accumulation of previous increments, thereby providing a permanent memory of damage orientation (Rots and Blaauwendraad, 1989).

The multi-directional crack model is a generalization of the fixed single crack model and allows for multiple cracks to form in a single sample point, just by decomposing the crack strain component in (2.8). The formulation follows similar lines as with the previous model, although with tensors of greater dimension. However, the issue of crack state changes becomes more cumbersome though traceable. Under conditions of tension-shear, the axes of principal stress rotate after crack formation, which leads to an increasing discrepancy between the axes of principal stress and the fixed crack axes (Rots and Blaauwendraad, 1989). Hence, the criterion to control formation of new cracks is to define a threshold angle for the angular deviation between the maximum principal stress and the normal to the last formed crack. Beyond this arbitrary threshold angle, a new crack is initiated.

The rotating crack model (RCM) enforces coaxiality of the axes of material orthotropy with the axes of principal strain throughout the incremental step, which justifies the use of nonlinear stress-strain curves that would otherwise partially lose physical meaning, since strain and stress tensors would no longer share eigenvectors. The coaxiality condition has direct consequences on the constitutive operator, the shear components of which have to have a certain form, as shown by Bažant (1983). Special provisions have to be made with these components if there is double or triple coincidence of principal strain values (Grassl and

Jirásek, 2006a). Provided that certain conditions are fulfilled (Rots, 1988), the rotating crack model can be conceived as the continuous counterpart to which the multi-directional model tends as the threshold angle approaches zero, thereby allowing to maintain strain decomposition.

The local constitutive operator relating local crack strains to local tractions can account for explicit shear-normal coupling through non-zero off-diagonal terms or include this effect implicitly, keeping a diagonal tensor structure but postulating relations between stiffness moduli and strains of different modes. Softening, as already noted, is defined at constitutive level (Fig. 2.10).

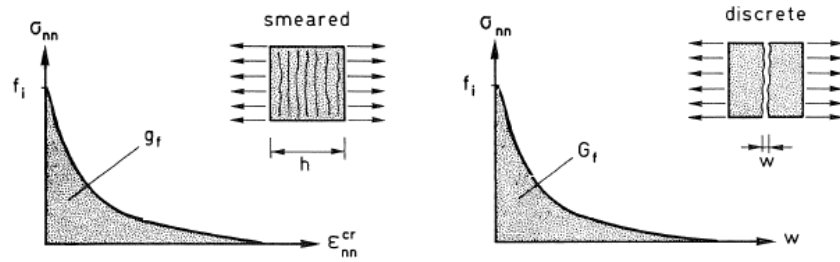


Figure 2.10: (left) Stress vs crack strain diagram (right) Stress vs crack opening diagram.

(Rots *et al.* 1985)

Figure 2.10 shows one of the main features of smeared cracking: fracture is assumed to be uniformly distributed over a crack bandwidth  $h$ , which under certain conditions (Rots *et al.* 1985) can be assumed to be equivalent to the crack band proposed in (Bažant and Oh, 1983). The crack bandwidth  $h$  is related to the particular finite element configuration (Rots and Blaauwendraad, 1989) and, if chosen appropriately, such that  $hg_f = G_f$ , the energy dissipated in fracture is the same regardless of the crack model and mesh refinement.

If  $h$  were not defined, since the constitutive laws are affected by softening, thereby changing the mathematical nature of the boundary value problem (loss of ellipticity of the differential equations leading to ill-posedness), the numerical outcome would display spurious mesh sensitivity, with strain localising into a narrow band whose width depends on the element size, tending to zero with mesh refinement. The total energy dissipated by fracture would converge to zero as well, which is physically unacceptable (Jirásek, 1998). Also, recalling from Section 2.3 that a dimensional analysis shows the need for a parameter with dimensions of length to complete the formulation, the role of  $h$  becomes apparent. It is needed to adjust

the stiffness modulus capturing softening at constitutive level so that fracture energy invariance is guaranteed (i.e. objectivity is ensured), and it constitutes a first step towards a non-local softening model (Section 2.6), a material formulation with internal length scales (Rots, 1988).

As elaborated in Rots and Blaauwendraad (1989), the relations between the crack stiffness moduli and the traditional softening continuum parameters are expressed as:

$$\frac{1}{\beta G} = \frac{1}{G} + \frac{1}{D''} \quad (2.11)$$

$$\frac{1}{\mu E} = \frac{1}{E} + \frac{1}{D'} \quad (2.12)$$

with  $\mu$  standing for the reduction factor of mode I stiffness and  $\beta$  standing for the shear retention factor (SRF), and  $E$  and  $G$  being the elastic moduli.  $D'$ ,  $D''$  and  $D'''$  are the diagonal terms of the local crack stiffness matrix relating increments of  $\mathbf{t}_c$  and  $\mathbf{e}_c$ . As illustratively shown in Figure 2.11, it is possible to specify an upper limit for bandwidth  $h$ , essentially linked to the avoidance of snap-back instability at local integration point level. If the crack band exceeds this limit, it becomes necessary to reduce the strength in combination with a sudden stress drop to maintain fracture energy invariance (Bažant, 1986) (Fig. 2.12).

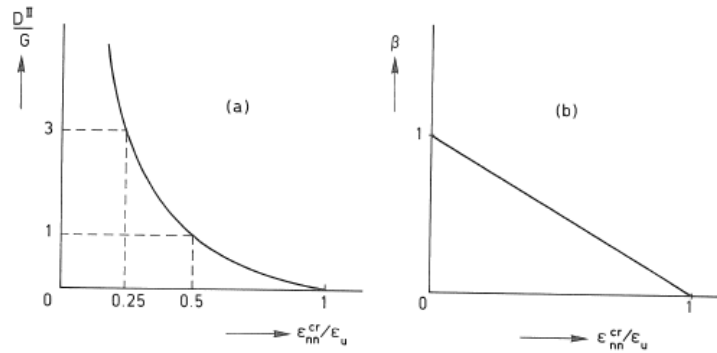


Figure 2.11: (a) Mode II shear modulus (b) Correspondent SRF  
(Rots and Blaauwendraad, 1989)

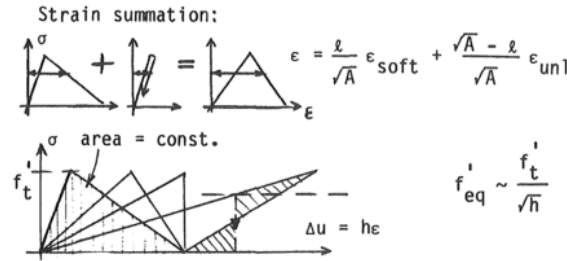


Figure 2.12: Adjustment of strength for distributed cracking (Bažant, 1986)

Qualitatively, a lower limitation for  $h$  has also been suggested (Bažant et al. 1984), leading to non-local continuum formulations (Section 2.6) for arbitrarily fine meshes. Determining  $h$ , however, is not always intuitive, although there are suggested simplifications to estimate it (Rots, 1988) or more consistent procedures to calculate it as a ratio of fracture energy  $G_f$  to specific energy  $g_f$  (Oliver, 1989).

All smeared crack models are formulated under the assumption that fracture is initiated in mode I. This is reasonable for materials with relatively large shear stiffness under predominantly tensile loading, which will generally fail in a (quasi)brittle manner with limited energy dissipation. In particular, the rotating crack model is essentially integrating a mechanism suited for brittle materials (crack initiation in mode I) with a concept rather characteristic of ductile materials (continuous rotation of failure orientation during damage) (Weihe, 1995). The latter is actually the reason behind the model not being able to preserve memory of damage, but the conjunction of both seems to capture well the dual behaviour of reinforced concrete, where crack initiation is governed by concrete quasi-brittleness but steel ductility is more relevant upon softening.

The smeared approach presents, however, a set of drawbacks. The fixed crack model does not control further rotated tensile stresses after crack formation, which, together with a non-zero stiffness parallel to the crack, might give rise to stresses beyond the tensile strength. This qualitative argumentation is one of the reasons behind the over-stiff response of smeared models in general, particularly the fixed crack one. Fig. 2.13 illustrates this point for a tension-shear test, whereby the threshold angle  $90^\circ$  corresponds to the fixed crack case.

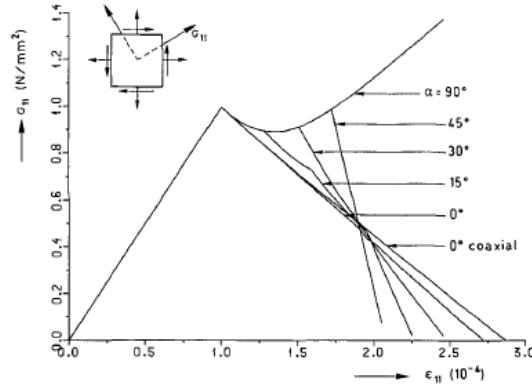


Figure 2.13: Principal stress-strain response for different threshold angles under tension-shear (Rots and Blaauwendraad, 1989)

Furthermore, the clash between the inherent displacement discontinuity of a discrete crack and the continuous representation of finite element interpolations leads to spurious stress transfer (stress locking), which in turn causes spurious cracking or spurious stiffening, depending on the locked stresses being greater than the tensile strength or the opposite, respectively. Figure 2.14 shows an example of this phenomenon affecting simulations of the Crack-Line-Wedge-Loaded Double-Cantilever-Beam (CLWL-DCB) tested by Kobayashi *et al.* (1985).

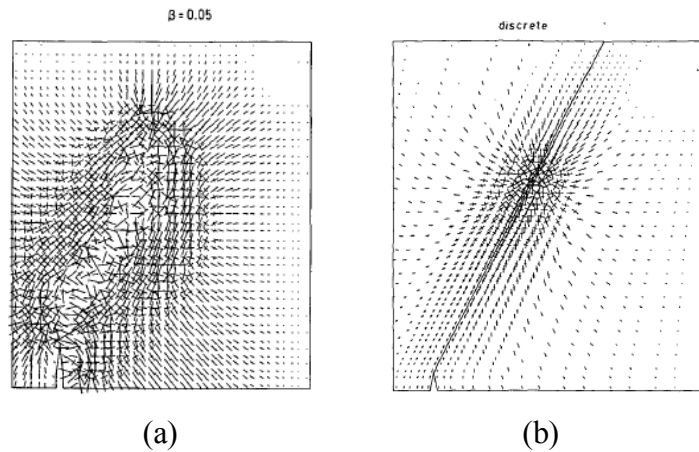


Figure 2.14: Principal tensile stress trajectories for (a) Fixed crack with SRF = 0.05  
(b) Discrete crack, from (Rots and Blaauwendraad, 1989)

A formal approach to this problem, as in (Jirásek and Zimmermann, 1998a), shows that finite element interpolations provide a too poor kinematic representation of the displacement field around an opening macroscopic crack, and that the misalignment of such a crack with the element sides inevitably gives rise to spurious stresses. These do not disappear on mesh

refinement, since mesh refinement does not remove the fundamental assumption of displacement compatibility (Rots, 1988).

Additionally, the rotating crack model is potentially prone to show undesirable numerical behaviour caused by material instability, in particular from the shear coefficients from the material stiffness matrix that have to be of a certain shape to enforce coaxiality. Figure 2.15 shows the equivalent shear retention factor retrieved a posteriori from a tension-shear model problem (Rots, 1988).

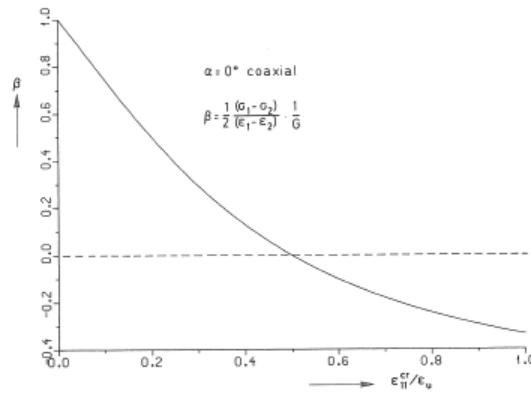


Figure 2.15: Development of equivalent SRF for coaxial rotating crack result  
(Rots and Blaauwendraad, 1989)

The shear material stiffness can thus become negative and potentially cause the model to lose stability by shear (Fig. 2.16) whenever the material softens in one direction and is subjected to tension in the perpendicular direction (Jirásek and Zimmermann, 1998b). The local instability might be alleviated at structural level through the stabilizing effect of neighbouring elements, but changing to non-local formulation increases the likelihood of this spurious kinematic mode destabilizing the analysis.

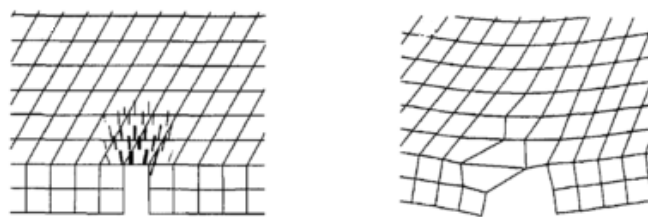


Figure 2.16: Unstable RCM simulation (left) Initial symmetric crack pattern (right) Instability mode (Jirásek and Zimmermann, 1998b)

## 2.4 Plasticity

Although treated separately, flow theory of plasticity as well as damage theories (Section 2.5) can be viewed as smeared approaches in the broad sense because they also comply with the notion of the material being a continuum at macro-scale. The differences arise in the particularities of the corresponding constitutive laws. For the specific case of concrete, the classical formulation of flow theory of plasticity can be found in Chen (1982). In essence, its three main pillars are the yield condition, the flow rule and the hardening law, to be complemented by the loading/unloading conditions.

Similar to (2.8) in crack models, strain can be decomposed into an elastic and a plastic component:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p \quad (2.13)$$

The yield condition is expressed by means of a yield function defined in stress space:

$$f_p(\boldsymbol{\sigma}, \boldsymbol{\kappa}) \leq 0 \quad (2.14)$$

whereby the stress state  $\boldsymbol{\sigma}$  is usually represented by invariants, and  $\boldsymbol{\kappa}$  stands for a vector collecting all internal variables. All points in stress space for which (2.14) is satisfied as a strict inequality refer to elastic states (leading to the initial yield surface also being called elastic envelope), and otherwise to plastic states. As shown in Jirásek and Bazant (2002), the stress dependent part of (2.14) that reflects reasonably the behaviour of concrete for the whole range of stresses is generically of the form:

$$c_1 \sigma_v + c_2 \rho r(\theta) + c_3 \rho^2 - 1 = 0 \quad (2.15)$$

where  $\{c_1, c_2, c_3\}$  are material parameters and  $\{\sigma_v, \rho, \theta\}$  are the coordinates associated to a cylindrical system with the hydrostatic axis as cylindrical axis (normally referred to as Haigh-Westergaard coordinates).

The direction of plastic flow is established with the flow rule:

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\partial g_p(\boldsymbol{\sigma}, \boldsymbol{\kappa})}{\partial \boldsymbol{\sigma}} \quad (2.16)$$

with  $\lambda$  as a scaling factor called plastic multiplier and function  $g_p$  as the plastic potential. Only for the particular case that  $f_p$  and  $g_p$  coincide is the flow rule called *associated*, with the direction of plastic flow perpendicular to the yield surface.

The hardening law:

$$\dot{\kappa} = \dot{\lambda} k(\sigma, \kappa) \quad (2.17)$$

describes the evolution of the internal variables, which in turn affects the evolution of the yield surface in stress space. Most commonly, the yield surface is scaled with respect to a reference point (isotropic hardening) or shifted without distortion (kinematic hardening).

The loading/unloading conditions are most concisely presented in the Karush-Kuhn-Tucker form:

$$\dot{\lambda} \geq 0, f_p \leq 0, \dot{\lambda} f_p = 0 \quad (2.18)$$

which formally restricts the plastic flow direction to follow the direction given by the plastic potential, the stress points to be inside or on the yield surface and the internal plastic variables to remain constant if the stress state is elastic.

Isotropic hardening has shown to capture reasonably well the behaviour of concrete under compressive states. Also, for realistic modelling of the volumetric expansion under low-confined compression observed in this kind of frictional materials, a non-associated flow rule is necessary. An associated flow rule gives rise to an unrealistically high dilation, which leads in certain cases to an overestimated strength (Grassl and Jirásek, 2006b; Grassl, 2004). If non-associativity is restricted to the volumetric part, e.g. in the extended Leon model (Etse and Willam, 1994), or if it is both volumetric and deviatoric but remains overall an isotropic scalar function of stresses, e.g. in certain damage-plastic models (Grassl *et al.*, 2013), then the gradient of the plastic potential (i.e. the plastic strain increment) still shares eigenvectors with the stresses at the end of the incremental step. Furthermore, it has been shown to be reasonable to accept that the total plastic strain has the same orientation as the plastic strain increment, at least for monotonic loading (Grassl *et al.*, 2002). Hence, in the frame of hardening plasticity, non-associated flow as described above can maintain macro-scale isotropy and thereby coaxiality of principal stresses and strains.

If softening is included in the plastic formulation, the problem becomes ill-posed and even local uniqueness might be lost, i.e. certain stress histories not being uniquely determined by the model equations, if the softening plastic modulus drops below a critical value (Grassl and Jirásek, 2006a).

As noted for the case of smeared crack softening, plastic softening needs an internal length parameter for regularisation purposes, normally inserted in the formulation of an internal variable  $\kappa_p$ , that adjusts the shape of the softening curve for energy dissipation invariance, otherwise lost in spurious mesh sensitivity. A more systematic approach for regularisation would be resorting to non-local models (Section 2.6), e.g. including the strain rate or gradients of  $\kappa_p$  in the formulation, or visco-plastic models (Valentini and Hofstetter, 2013). Stress locking (Section 2.3.3) is also a potential drawback because its formal causes are still present in softening plasticity (poor kinematic description unless the normal to the maximum principal stress and element side are aligned).

Most frequently, the evolution law for a hardening/softening parameter  $\kappa_p$ , contained in vector  $\mathbf{k}$  in (2.17), depends on the norm of the plastic strain rate scaled by factors that depend on the stress state, although there are alternatives that just consider the volumetric part of the plastic strain with no scaling that have provided good results for compressive stress states, as in Grassl *et al.* (2002).

A common generalisation of (2.14)-(2.17) consists of resorting to a combination of multiple yield surfaces, to accommodate the differences in the material response in different stress regions. Such approach is called multi-surface plasticity, leading to the so-called Koiter's generalisation as the following linear combinations of the yield condition, flow rule and hardening law, respectively (Koiter, 1953):

$$f_{p,i}(\boldsymbol{\sigma}, \boldsymbol{\kappa}) \leq 0 \quad (2.19)$$

$$\dot{\boldsymbol{\varepsilon}}_p = \sum_{i=1}^{S^a} \dot{\lambda}_i \frac{\partial g_{p,i}(\boldsymbol{\sigma}, \boldsymbol{\kappa})}{\partial \boldsymbol{\sigma}} \quad (2.20)$$

$$\dot{\boldsymbol{\kappa}} = \sum_{i=1}^{S^a} \dot{\lambda}_i \mathbf{k}_i(\boldsymbol{\sigma}, \boldsymbol{\kappa}) \quad (2.21)$$

$S^a$  stands for the number of active yield surfaces from the total set (i.e. those satisfying (2.19) as a strict equality), which in general is not known in advance and has to be determined iteratively. Existing multi-surface models for concrete can be found for example in the works of Feenstra and de Borst (1996) and Haufe (2001).

From the computational perspective, an evaluation algorithm is required to compute the stresses during the incremental-iterative procedure at global level. At a certain step  $(n)$ , a prescribed increment of strain (of which the split into elastic and plastic components is not known *a priori*) induces changes in the values of the remainder of state variables for step  $(n+1)$ . These can be obtained by solving (2.14), (2.16)-(2.17) for single-surface plasticity or (2.19)-(2.21) for multi-surface plasticity, along with the elastic constitutive relation and the loading/unloading conditions, giving rise to the updated stresses:

$$\boldsymbol{\sigma} = \mathbf{D}_e : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p) \quad (2.22)$$

The most widespread approach to integrating the rate form of the constitutive equations is by considering finite incremental steps and the following local residual system:

$$\begin{aligned} \mathbf{r}_\sigma &= \boldsymbol{\sigma}^{(n+1)} - \boldsymbol{\sigma}^{tr} + \Delta\lambda^{(n+1)} \mathbf{D}_e : \frac{\partial g_p(\boldsymbol{\sigma}^{(n+1)}, \boldsymbol{\kappa}^{(n+1)})}{\partial \boldsymbol{\sigma}} \\ \mathbf{r}_\kappa &= \boldsymbol{\kappa}^{(n+1)} - \boldsymbol{\kappa}^{(n)} - \Delta\lambda^{(n+1)} \mathbf{k}(\boldsymbol{\sigma}^{(n+1)}, \boldsymbol{\kappa}^{(n+1)}) \\ r_f &= f_p(\boldsymbol{\sigma}^{(n+1)}, \boldsymbol{\kappa}^{(n+1)}) \end{aligned} \quad (2.23)$$

initially assuming for each residual that the strain increment is fully elastic ( $\Delta\lambda^{(n+1)} = 0$ ). The corresponding stresses (called trial stresses  $\boldsymbol{\sigma}^{tr}$ ) lie outside the boundaries of the yield surface (2.14) if the assumption is incorrect, and an iterative procedure (e.g. following a Newton scheme, as in de Borst *et al.* (2012)) is required to find the admissible combination of elastic and plastic strains that satisfies (2.14) strictly, i.e. the combination of state variables that makes all residuals fall below a tolerance close to zero. The geometric notion of ‘pulling’ the stress point back to the yield surface is the reason behind denominating this evaluation algorithm stress-return algorithm. It is common to refer to the trial stress as elastic predictor and the return to the yield surface as plastic corrector. Furthermore, for the case that all involved gradients are evaluated at the end of step  $(n+1)$ , the implicit method is called Euler backward, as opposed to explicit Euler forward if the gradient evaluation is kept at step  $(n)$ . Other stress-return schemes are possible, like the Generalised Cutting Plane (GCP) algorithm (Simo and Ortiz, 1985), which is explicit but may become unstable if the incremental step size is not sufficiently small.

Plasticity-based models are naturally capable of capturing inelastic strains upon unloading. However, they do not properly describe the loss of stiffness observed in experiments. This problem becomes especially severe at large stages of the degradation process when the (smeared) crack is stress free and, according to plastic formulation, a reversal of the opening rate immediately generates a compressive traction, which is not physical (Jirásek and Zimmermann, 2001).

## 2.5 Damage

Damage mechanics models can be regarded as the counterpart to the plasticity based models of the previous section. They are based on a gradual degradation of the elastic stiffness tensor, which readily captures the stiffness degradation observed for tensile and low confined compressive loading in concrete. However, they fail to describe irreversible deformations. Continuum damage model formulations for concrete can be found in Mazars and Pijaudier-Cabot (1989). In general, the relation between stresses and strains can be expressed by means of a secant stiffness tensor:

$$\boldsymbol{\sigma} = \mathbf{D}_s : \boldsymbol{\varepsilon} \quad (2.24)$$

dependent on damage-driving internal variables of different order, from scalars to fourth order tensors (de Borst *et al.*, 2012; Lemaitre and Chaboche, 1990). Isotropic models are based in their simplest form on a single scalar function, whereas anisotropic models use damage tensors.

Formally, damage can be formulated in a similar manner to plasticity based models. A history dependence via internal variables is expressed by means of a damage loading function:

$$f_d(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}, \boldsymbol{\kappa}) \leq 0 \quad (2.25)$$

Although the function in (2.25) is most generic, usually damage models are strain-based, which allows for an explicit forward evaluation of stresses, instead of the iterative implicit backward Euler scheme typically applied in plasticity-based models. Basic scalar isotropic damage models depend on a single damage parameter  $\omega$  and assume that Poisson ratio at the continuum macro-scale does not change throughout the degradation process, leading to the following secant stiffness:

$$\mathbf{D}_s = (1 - \omega) \mathbf{D}_e \quad (2.26)$$

Resorting to a scalar measure of the strain level through an equivalent strain  $\tilde{\varepsilon}(\boldsymbol{\varepsilon})$  for this case further simplifies (2.25) to:

$$f_d(\tilde{\varepsilon}, \kappa_d) \equiv \tilde{\varepsilon} - \kappa_d \leq 0 \quad (2.27)$$

The proposed expressions in Mazars and Pijaudier-Cabot (1989) and de Vree *et al.* (1995) (also known as Rankine and modified von Mises definitions, respectively) are amongst the more common definitions of equivalent strain for quasi-brittle materials, although more recent alternatives are also possible (Häußler-Combe and Pröchtel, 2005). An evolution law  $\omega(\kappa_d)$  dictating damage growth (usually linear, bilinear or exponential) along with the Karush-Kuhn-Tucker conditions for loading/unloading:

$$\dot{\kappa}_d \geq 0, f_d \leq 0, \dot{\kappa}_d f_d = 0 \quad (2.28)$$

complete the formulation for the scalar isotropic damage case.

All components of the material stiffness tensor decay to zero, proportionally to  $(1 - \omega)$ , and so do all stress components consequently. Hence, isotropic damage models do not transfer spurious stresses across a widely open crack and thereby constitute an exception within smeared softening models where stress-locking does not occur (Jirásek and Zimmermann, 1998b).

Anisotropic damage models generalise (2.26) by expressing the constitutive relation as (Lemaitre and Chaboche, 1990):

$$\boldsymbol{\sigma} = (\mathbf{I} - \boldsymbol{\Omega}) : \mathbf{D}_e : \boldsymbol{\varepsilon} \quad (2.29)$$

where  $\mathbf{I}$  and  $\boldsymbol{\Omega}$  are the unit fourth order tensor and the damage tensor, respectively. Alternatively, (2.29) can be more concisely expressed as (Jirásek, 2014):

$$\boldsymbol{\sigma} = \mathbf{M}^{-1} : \mathbf{D}_e : \boldsymbol{\varepsilon} \quad (2.30)$$

with the damage effect tensor  $\mathbf{M}$ . Due to the difficulty in prescribing evolution laws for the components of fourth order tensors that can be separately reflected in experiments, it is preferred to describe the damage effect by symmetric second order tensors, as introduced by Murakami (1983). Although this simplification entails restraining general anisotropy to orthotropy, it is considered to suffice for the description of the material response of concrete, which tends towards orthotropy for predominantly tensile stress states but remains closer to isotropy for compressive stress states (Lemaitre and Chaboche, 1990).

## 2.6 Regularisation

As commented in Section 2.3.2, constitutive strain softening formulations lead to ill-posed problems displaying spurious mesh-dependency of the localisation of inelastic strains and dissipated energy. A remedy to this can be obtained by a suitable regularisation technique, enforcing mesh-independent dissipation associated with the failure process (Grassl and Jirásek, 2006b). The resulting enriched continuum formulation is called non-local and is readily applicable to plasticity as well as damage based models. This non-locality can be achieved via weighted spatial averaging (integral-type) or incorporating higher order gradients into the constitutive model (differential type). The state or internal variable to be non-locally formulated is arbitrary but it has to be chosen carefully because certain non-local formulations are inherently incapable of reproducing the entire material degradation process up to complete failure (Jirásek, 1998). Most frequently, non-local formulations are based on strains or internal parameters representing equivalent strains.

All non-local models incorporate a characteristic length parameter in their formulation that sets the internal length scale discussed in Section 2.3.2. For integral type of non-locality, this parameter is typically called  $R$ , radius of non-local interaction.

Attention must be paid when non-local models deal with localised inelastic strains near boundaries, e.g. the notch in a three-point bending test. It affects the spatial averaging procedure and shifts the maximum inelastic strains to a certain distance of the notch tip (Jirásek and Rolshoven, 2003), which can have a significant influence at structural level with plastic-damage models (Grassl, 2009).

## 2.7 Combined approaches

In the framework of the smeared approach, all the material modelling alternatives reviewed hitherto are considered separately for illustration purposes, but combinations between them are feasible and indeed advantageous. To this end, two combined approaches are taken in consideration hereafter.

### 2.7.1 Damage and plasticity

Damage and plasticity are smeared formulations that complement each other conveniently. Plasticity accounts for irreversible deformations, path dependency and the ductile hardening

behaviour observed in highly confined compression states, whereas damage can capture the reduction of unloading stiffness and also the characteristic softening of tensile and low confined compressive states.

There are various combined models of this nature in the literature (Lubliner *et al.*, 1989; Oller *et al.*, 1996). One of the most widely spread relies on combining stress-based plasticity in the effective (undamaged) stress-space with a strain-based scalar damage model, as in Grassl *et al.* (2013) or Grassl and Jirásek (2006a) , with the name concrete damage-plastic model (CDPM2 or CDPM). Although the latter model with a single damage parameter has shown to describe monotonic loading with unloading satisfactorily, the former model, using two separate isotropic damage variables for tension and compression, seems better suited for modelling the transition from tensile to compressive failure realistically (Grassl *et al.*, 2013) .

Plasticity and damage are also coupled in (Leukart, 2005) within the frame of micro-plane modelling, which naturally allows for anisotropic formulation. Micro-plane theory has not been reviewed in previous sections deliberately because, although part of continuum-based constitutive descriptions, its formulation is developed in a ‘lower’ reference level, a micro-plane level with strain vectors kinematically constrained to the macro strain-tensor and stress vectors obtained via weak formulation. Its philosophy (angular discretization with respect to orientation) blends well with finite element modelling (spatial discretization with respect to distance) and also with the non-local concept (captures interactions of damage at distance while micro-plane captures interactions among angular orientations) (Jirásek and Bazant, 2002). However, although this model does not resort directly to meso-scale, it represents a two-way switch between macro- and lower scales that requires inverse analysis for estimation of additional parameters, and its efficiency at structural level remains questionable.

### **2.7.2 Fracture and plasticity**

There are several publications dealing with plasticity-based as well as smeared-crack material models for concrete. Combinations of both approaches are less numerous in the literature, one of the earliest references being (de Borst, 1986), with more recent revisions like (Červenka and Papanikolaou, 2008).

In the model proposed by Červenka and Papanikolaou, the fracture part of the model provides the expected anisotropic behaviour upon cracking (as smeared orthotropy) whereas the plastic part, based on non-associativity and a hardening-softening parameter dependent on the volumetric component of the plastic strain, depicts compressive crushing. The plastic potential maintains dependency on the third invariant, usually neglected for reasons of implementation efficiency and model robustness, thereby allowing for a better description of multiaxial compressive responses.

The main computational advantages arise from the strain decomposition in fracture and plastic components, the formal similarity in the basic structure of both equation systems and the entirely separate solution algorithms. Within the fracture part, attention is focused on shear behaviour after cracking. Formulation of shear crack stiffness parameters for modes II and III follows from intuitive relations with the mode I crack opening law. The treatment given by Rots (1988) to these coefficients – for the case of multi-directional cracks with a threshold angle - seems better suited since it allows for implicit coupling between modes. Also, it is argued by the authors that the compressive strength of cracked concrete should be reduced upon crack opening in other directions to better fit experimental data. This could be done by relating parameters of both parts, but the coupling would complicate the solution algorithm, thereby losing computational efficiency.

## **2.8 Conclusions**

Several alternatives for the material modelling of concrete fracture have been presented and reviewed, mainly distinguishing between discrete and smeared (in the broad sense) approach. The former more intuitively introduces a discontinuity in displacement, corresponding to the physical separation that a crack introduces in a fracturing body, without entering the constitutive level. The latter, on the contrary, maintains the continuum nature of the formulation, as a natural transition from elasticity, at the cost of affecting the constitutive relations. Several advantages and drawbacks are pointed out for each approach, with emphasis on the increase in the size of the discretised system, potential re-meshing, stress locking and need for an internal length scale. In light of these, and considering the main aim of computational performance at larger scale as well as the potential inclusion of reinforcement, it is decided to focus on the smeared approach set of models.

The combined damage-plastic and fracture-plastic models are considered as potential candidates for implementation, whereby the former belongs to single-surface plasticity and the latter is analogous to a multi-surface plasticity model.

As commented in Section 2.5, scalar damage is the only alternative within smeared softening approaches which can ensure that no spurious stresses are transferred across an open crack. Hence, stress locking is a relevant issue for the fracture-plastic model, either with fixed or rotating crack representation.

As reviewed further in Chapter 3, the achievement of a quadratic convergence rate at global level (by means of a full Newton-Raphson scheme) necessitates the calculation of the tangential moduli (algorithmic stiffness) consistent with the appropriate stress update algorithm. The fracture-plastic model resorts to a modified Newton-Raphson scheme, calculating the secant stiffness, which only allows for linear convergence rate. Additionally, certain stress states may lead to all surfaces (plastic yield surface and fracture cut-offs) being simultaneously active and returned stress states located in the sharp corners of their intersection in stress space. Consequently, the potential derivation of the algorithmic stiffness for these cases becomes more cumbersome.

The damage-plastic model CDPM/CDPM2, on the other hand, comprises a convex smooth surface with no gradient discontinuities except in the intersections with the hydrostatic axis. From the two versions of the damage-plastic model, only the original one (CDPM) can accommodate the consistent derivation of the algorithmic stiffness, since the later version (CDPM2) defines compressive damage via an implicit equation that does not allow explicit differentiation. Furthermore, CDPM2 introduces linear hardening in the plastic yield surface after onset of damage, as opposed to CDPM where the yield surface remains fixed in stress space with active damage. Although the inclusion of linear hardening at post-peak has advantages in terms of mesh independence of the plastic strain profile, the fixity of the yield surface entails significant benefits in terms of algorithmic robustness.

CDPM2 and the fracture-plastic model are able to capture responses under load sign reversal or cyclic loading. The latter accommodates this naturally as the fracture cut-offs are associated to tensile states and the plastic yield function to compressive states, each with a different load function linked to a different internal variable history. CDPM2 splits the

damage part into tensile and compressive components, giving rise to two scalar damage variables and six strain-like internal variables, as opposed to CDPM where only one variable of each type is necessary. In this case, however, history of damage is constrained and no distinction between stress states can be made, leading to a spurious damage memory upon load sign reversal.

In light of all the aforementioned aspects, and notwithstanding some of its aforementioned shortcomings, CDPM is chosen as the model to be implemented and enhanced in the following chapters.

# CHAPTER 3

## Modelling of concrete

### 3.1 Introduction

As described in Chapter 2, the current Chapter aims at introducing the main features of the Concrete Damage-Plastic Model (CDPM) proposed by Grassl and Jirásek (2006a) and selected as material model in the framework of this thesis. After a brief summary of the main mathematical components in both the plastic and the damage parts of the CDPM, and a proposed new extension of the latter to an anisotropic version, focus is placed on the algorithmic architecture proposed for its implementation, which comprises novel enhancements, justified and thoroughly elaborated in Section 3.3.1. Subsequently, the enhanced model is verified in Section 3.3.2 by means of numerical tests that corroborate its improved numerical robustness, and an additional modification to reconcile the hydrostatic response on different planes is discussed in this context in Section 3.3.3. The consistent algorithmic stiffness is derived for both the isotropic and the anisotropic version of the CDPM in Section 3.4, including new provisions for limiting cases hindering its definition. Additionally, the directional properties of the CDPM are investigated and assessed via localisation analysis in Section 3.5. Finally, a regularisation scheme to ensure mesh objectivity is reviewed and discussed in Section 3.6.

## 3.2 Description of CDPM material model

The formulation of the selected material model as presented hereafter allows for a separate treatment of plasticity and damage, which also has significant benefits from the implementation perspective. Hence, the two distinct parts of the model are also presented separately, whereby the linking variables coupling them are duly highlighted. Following the original notation by Grassl and Jirásek (2006a), the undamaged (*effective*) variables intervening in the plastic part are denoted with an overhead bar (e.g.  $\bar{\sigma}$ ), whereas their damaged (*nominal*) counterparts dispense with it (e.g.  $\sigma$ ). Tensorial notation is used throughout by default, whilst resorting to vectorial notation is explicitly remarked, where appropriate.

### 3.2.1 Plastic part

Plasticity is formulated in the effective stress space, by means of a single smooth convex yield surface, in turn expressed in terms of the effective Haigh-Westergaard coordinates (volumetric stress  $\bar{\sigma}_v$ , deviatoric radius  $\bar{\rho}$  and Lode angle  $\bar{\theta}$ ) and an internal strain-like variable ( $\kappa_p$ ). The Haigh-Westergaard coordinates form a cylindrical reference system in the principal effective stress space, with the hydrostatic axis as the cylindrical axis, and are defined as:

$$\bar{\sigma}_v = \frac{I_1}{3} \quad (3.1)$$

$$\bar{\rho} = \sqrt{2J_2} \quad (3.2)$$

$$\bar{\theta} = \frac{1}{3} \arccos\left(\frac{3\sqrt{3}}{2} \frac{J_3}{\sqrt{J_2^3}}\right) \quad (3.3)$$

where  $I_1$  is the first effective stress invariant, and  $J_2$  and  $J_3$  are the second and third deviatoric effective stress invariants, respectively:

$$\begin{aligned} I_1 &= \bar{\sigma} : \delta \\ J_2 &= \frac{1}{2} \bar{\mathbf{s}} : \bar{\mathbf{s}} \\ J_3 &= \frac{1}{3} \bar{\mathbf{s}}^3 : \delta \end{aligned} \quad (3.4)$$

$\delta$  stands for the Kronecker delta,  $\bar{s}$  for the effective deviatoric stress tensor and the colon symbol for the double contraction operation. The coordinate surface corresponding to a constant value of  $\bar{\theta}$  is a meridian plane, and the curve resulting from its intersection with the yield surface is called meridian. The yield function:

$$f_p(\bar{\sigma}_V, \bar{\rho}, \bar{\theta}, \kappa_p) = \left\{ (1 - q_h(\kappa_p)) \left( \frac{\bar{\rho}}{\sqrt{6}\bar{f}_c} + \frac{\bar{\sigma}_V}{\bar{f}_c} \right)^2 + \sqrt{\frac{3}{2}} \frac{\bar{\rho}}{\bar{f}_c} \right\}^2 + m_0 q_h^2(\kappa_p) \left( \frac{\bar{\rho}}{\sqrt{6}\bar{f}_c} r(\cos \bar{\theta}) + \frac{\bar{\sigma}_V}{\bar{f}_c} \right) - q_h^2(\kappa_p) \quad (3.5)$$

is a modification of the Extended Leon Model developed by Etse and Willam (1994), whereby the Willam and Warnke (1975) function:

$$r(\cos \bar{\theta}) = \frac{4(1 - e^2) \cos^2 \bar{\theta} + (2e - 1)^2}{2(1 - e^2) \cos \bar{\theta} + (2e - 1) \sqrt{4(1 - e^2) \cos^2 \bar{\theta} + 5e^2 - 4e}} \quad (3.6)$$

controlling the shape of the deviatoric section affects here only the linear term of the deviatoric radius. Following the explicit definition of the eccentricity parameter suggested by Jirásek and Bazant (2002):

$$e = \frac{1 + \psi}{2 - \psi} \quad (3.7)$$

$$\psi = \frac{\bar{f}_t}{\bar{f}_c} \frac{\bar{f}_b^2 - \bar{f}_c^2}{\bar{f}_c^2 - \bar{f}_t^2}$$

where parameters  $\bar{f}_c$ ,  $\bar{f}_t$  and  $\bar{f}_b$  denote the uniaxial compressive and tensile strength and the equibiaxial compressive strength, respectively, allows the natural transition of the yield function's deviatoric shape to occur with a constant eccentricity parameter. This transition evolves from triangular to circular along the hydrostatic axis, tending towards the latter as confinement increases, as opposed to the original expression proposed by Etse and Willam (1994) where  $e$  would depend on the volumetric stress.

The friction parameter  $m_0$  depends on the strength values as well as on the eccentricity:

$$m_0 = 3 \frac{\bar{f}_c^2 - \bar{f}_t^2}{\bar{f}_c \bar{f}_t} \frac{e}{e + 1} \quad (3.8)$$

By denoting  $R_f$  as the ratio of tensile to compressive strength, it is possible to reformulate (3.8) as:

$$m_0 = \frac{(1 - R_f^2)}{R_f} \left( \frac{3e}{e+1} \right) \quad (3.9)$$

Since for concrete it is generally applicable that  $\bar{f}_b > \bar{f}_c$  and that  $\bar{f}_c > 6\bar{f}_t$ , leading to  $\psi \neq 0$  and  $e > \frac{1}{2}$ , the second term in the right hand side of (3.9) introduces an augmentative correction to the decay of  $m_0$  with the ratio of strength values.

Incidentally, the above inequalities also guarantee the thermodynamic consistency of the model by satisfying the dissipation inequality, as elaborated upon in Grassl and Jirásek (2006a). The friction parameter  $m_0$  and the normalised variable  $q_h$  (in turn dependent on  $\kappa_p$ ) define the shape of the meridians, which are parabolic (Figure 3.1).

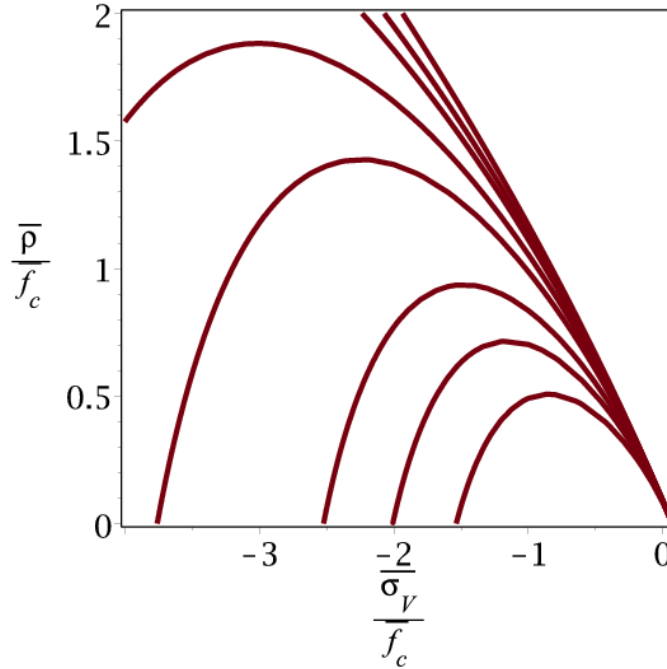


Figure 3.1: Evolution of the normalized meridians for  $\bar{\theta} = 0$  from the elastic envelope ( $q_h = q_{h0}$ ) to the final hardened state ( $q_h = 1$ )

The normalised hardening variable  $q_h$  attains a maximum value of 1 starting from  $q_{h0}$ , representing a nonlinear isotropic hardening process at the end of which the yield surface becomes the Menétrey and Willam (1995) failure surface:

$$f_p(\bar{\sigma}_v, \bar{\rho}, \bar{\theta}, \kappa_p \geq 1) = \frac{3}{2} \left\{ \frac{\bar{\rho}}{f_c} \right\}^2 + m_0 \left( \frac{\bar{\rho}}{\sqrt{6}f_c} r(\cos \bar{\theta}) + \frac{\bar{\sigma}_v}{f_c} \right) - 1 \quad (3.10)$$

The plastic flow rule is non-associated and defined by:

$$\dot{\boldsymbol{\varepsilon}}_p = \dot{\lambda} \frac{\partial \mathbf{g}_p}{\partial \boldsymbol{\sigma}} = \dot{\lambda} \mathbf{m} \quad (3.11)$$

with the plastic potential given as:

$$g_p(\bar{\sigma}_V, \bar{\rho}, \kappa_p) = \left\{ (1 - q_h(\kappa_p)) \left( \frac{\bar{\rho}}{\sqrt{6}\bar{f}_c} + \frac{\bar{\sigma}_V}{\bar{f}_c} \right)^2 + \sqrt{\frac{3}{2}} \frac{\bar{\rho}}{\bar{f}_c} \right\}^2 + q_h^2(\kappa_p) \left( \frac{m_0 \bar{\rho}}{\sqrt{6}\bar{f}_c} + \frac{m_g(\bar{\sigma}_V)}{\bar{f}_c} \right) \quad (3.12)$$

and its gradient represented by  $\mathbf{m}$ . The quadratic terms of the yield function remain unchanged in the plastic potential, with the differences between both functions arising from the linear terms, where the deviatoric radius is left unaffected by the Willam and Warnke function (3.6). This independence of Lode's angle implies that the plastic potential becomes a set of revolution surfaces around the hydrostatic axis, giving rise to radial returns along a fixed meridian plane. Additionally, the shape of the meridians of the plastic potential is now controlled by:

$$m_g(\bar{\sigma}_V) = A_g B_g \bar{f}_c \exp \left( \frac{\bar{\sigma}_V - \frac{\bar{f}_t}{3}}{B_g \bar{f}_c} \right) \quad (3.13)$$

where  $A_g$  and  $B_g$  are model parameters given by:

$$A_g = \frac{3\bar{f}_t}{\bar{f}_c} + \frac{m_0}{2} \quad (3.14)$$

$$B_g = \frac{\frac{1}{3} \left( 1 + \frac{\bar{f}_t}{\bar{f}_c} \right)}{\ln A_g - \ln(2D_f - 1) - \ln \left( 3 + \frac{m_0}{2} \right) + \ln(D_f + 1)} \quad (3.15)$$

and the dilation ratio is  $D_f = 0.85$  as it provides good agreement with experimental results.

From all the above, it follows that non-associativity is both volumetric and deviatoric. The hardening law is given by:

$$q_h(\kappa_p) = \begin{cases} q_{h0} + (1 - q_{h0}) \kappa_p (\kappa_p^2 - 3\kappa_p + 3) & \text{if } \kappa_p < 1 \\ 1 & \text{if } \kappa_p \geq 1 \end{cases} \quad (3.16)$$

with  $C^1$  continuity achieved at  $\kappa_p = 1$ . The evolution law of the internal strain-like hardening variable:

$$\dot{\kappa}_p(\bar{\sigma}, \kappa_p) = \frac{\|\dot{\epsilon}_p\|}{x_h(\bar{\sigma}_V)} (2 \cos \bar{\theta})^2 = \frac{\dot{\lambda} \|\mathbf{m}\|}{x_h(\bar{\sigma}_V)} (2 \cos \bar{\theta})^2 = \dot{\lambda} k_p(\bar{\sigma}, \kappa_p) \quad (3.17)$$

is linked to the evolution of the norm of the plastic strain rate  $\|\dot{\epsilon}_p\|$  along a fixed meridian plane, modulated by a ductility parameter  $x_h$ :

$$x_h = \begin{cases} A_h - (A_h - B_h) \exp(-R_h(\bar{\sigma}_V)/C_h) & \text{if } R_h(\bar{\sigma}_V) \geq 0 \\ E_h \exp(R_h(\bar{\sigma}_V)/F_h) + D_h & \text{if } R_h(\bar{\sigma}_V) < 0 \end{cases} \quad (3.18)$$

$$R_h(\bar{\sigma}_V) = -\frac{\bar{\sigma}_V}{f_c} - \frac{1}{3} \quad (3.19)$$

that slows down hardening evolution with increasing confinement.  $A_h$  to  $F_h$  are model parameters to be calibrated as described in Grassl and Jirásek (2006a).

### 3.2.2 Damage part

Although formally there is a damage loading function expressed in the strain space as follows:

$$f_d(\epsilon, \epsilon_p, \kappa_d) = \tilde{\epsilon}(\epsilon, \epsilon_p) - \kappa_d \quad (3.20)$$

with  $\tilde{\epsilon}$  being the equivalent strain and  $\kappa_d$  being an internal strain-like damage-driving variable,  $\tilde{\epsilon}$  is not defined explicitly but rather incrementally:

$$\dot{\tilde{\epsilon}} = \begin{cases} 0 & \text{if } \kappa_p < 1 \\ \frac{\dot{\epsilon}_{pV}}{x_s(\bar{\sigma}_V)} & \text{if } \kappa_p \geq 1 \end{cases} \quad (3.21)$$

where  $\dot{\epsilon}_{pV}$  is the volumetric part of the plastic strain rate, and  $x_s$  is a softening ductility factor that, analogously to  $x_h$ , slows down evolution of the strain-like damage-driving variable for increasing confinement. It is worth noting that the coupling between the plastic and damage parts lies herein, as it is the evolution of the volumetric plastic strain (potentially reduced by  $x_s$ ) that dictates the evolution of the equivalent strain once the threshold marking

the end of hardening ( $\kappa_p = 1$ ) has been surpassed. Following a later version of CDPM by Grassl *et al.* (2013),  $x_s$  is calculated as an explicit function of the effective stress:

$$x_s = 1 + (A_s - 1)R_s \quad (3.22)$$

$$R_s = \begin{cases} -\frac{\sqrt{6}\bar{\sigma}_v}{\bar{\rho}} & \text{if } \bar{\sigma}_v \leq 0 \\ 0 & \text{if } \bar{\sigma}_v > 0 \end{cases} \quad (3.23)$$

with  $A_s = 15$  as a recommended value in Grassl and Jirásek (2006a) in the absence of experimental data.

Damage is isotropic and defined by a single scalar parameter  $\omega$ , which in turn controls a softening law of exponential form:

$$\omega = g_d(\kappa_d) = 1 - \exp\left(-\frac{\kappa_d}{\varepsilon_f}\right) \quad (3.24)$$

where  $\varepsilon_f$  is a parameter that controls the initial slope of the softening diagram and is determined from the fracture energy and a certain characteristic element size, hence contributing to regularization in localized failure modes (see Section 3.6). Since damage can only evolve upon activation of the damage loading function (3.20),  $\kappa_d$  in (3.24) represents directly the equivalent strain (i.e.  $f_d = 0$ ). Finally, the nominal (damaged) stresses are calculated from the effective stresses as:

$$\boldsymbol{\sigma} = (1 - \omega)\bar{\boldsymbol{\sigma}} = (1 - \omega)\mathbf{D}_e : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p) \quad (3.25)$$

where  $\mathbf{D}_e$  is the elastic stiffness, and  $\boldsymbol{\varepsilon}$  and  $\boldsymbol{\varepsilon}_p$  are total and plastic strain, respectively.

Alternatively, it is proposed here to generalise the damage part as anisotropic which, as commented in Chapter 2, is more suitable for reflecting multiaxial tensile states. To this end, the damage loading function (3.20) is generalised to:

$$f_d = g_d(\tilde{\boldsymbol{\varepsilon}}) - \boldsymbol{\delta} : \boldsymbol{\omega} \quad (3.26)$$

where  $g_d$  is the same exponential law as in (3.24). The definition of equivalent strain  $\tilde{\boldsymbol{\varepsilon}}$  remains unaffected but the scalar parameter  $\omega$  (3.24) becomes a second order tensor  $\boldsymbol{\omega}$  in (3.26), allowing for different damage components for different orientations. Hence, the

strain-like damage-driving variable evolving upon activation of the damage loading function (3.26) is the *trace* of  $\boldsymbol{\omega}$ , i.e. a ‘volumetric’ damage that effectively plays the same formal role as  $\kappa_d$  in the isotropic model. Based on (Desmorat *et al.*, 2010; Desmorat *et al.*, 2007), the rate form of the damage tensor is postulated as:

$$\dot{\boldsymbol{\omega}} = \dot{\lambda}_d \boldsymbol{\epsilon}_p^2 \quad (3.27)$$

The squares of plastic strains (3.11) as obtained from the plastic part dictate the rate of damage, scaled by a damage multiplier  $\lambda_d$  similarly to its plastic counterpart scaling the gradient of the plastic potential in (3.11). Originally, Desmorat *et al.* linked the damage rate form (3.27) to the positive part of total strains  $\langle \boldsymbol{\epsilon} \rangle^2$  instead, but the current rate form is preferred as it is consistent with the equivalent strain definition and allows to further link the plastic and damage parts. Moreover, the coaxiality between tensors arising from (3.27) entails implementation benefits, as the working space is that of principal stresses and strains. After integration of the damage rate form (3.27) as described in Section 3.3, and defining the auxiliary tensor:

$$\tilde{\boldsymbol{\omega}} = (\boldsymbol{\delta} - \boldsymbol{\omega})^{1/2} \quad (3.28)$$

where  $\tilde{\boldsymbol{\omega}}$  shares Eigenvectors with  $\boldsymbol{\omega}$  and has Eigenvalues  $\tilde{\omega}_i = \sqrt{1 - \omega_i}$ , the nominal stresses are finally obtained as:

$$\boldsymbol{\sigma} = \tilde{\boldsymbol{\omega}} \cdot \bar{\boldsymbol{\sigma}} \cdot \tilde{\boldsymbol{\omega}} \quad (3.29)$$

with the single dot standing for single contraction. For ease of comparison with the isotropic expression (3.25), in principal axes of damage (3.29) can be developed as:

$$\begin{aligned} (1 - \omega_1) \bar{\sigma}_{11} &= \sigma_{11} \\ (1 - \omega_2) \bar{\sigma}_{22} &= \sigma_{22} \\ (1 - \omega_3) \bar{\sigma}_{33} &= \sigma_{33} \\ \sqrt{(1 - \omega_1)(1 - \omega_2)} \bar{\sigma}_{12} &= \sigma_{12} \\ \sqrt{(1 - \omega_1)(1 - \omega_3)} \bar{\sigma}_{13} &= \sigma_{13} \\ \sqrt{(1 - \omega_2)(1 - \omega_3)} \bar{\sigma}_{23} &= \sigma_{23} \end{aligned} \quad (3.30)$$

### 3.3 Novel solution algorithm

The damage part is computed explicitly once the effective stresses  $\bar{\boldsymbol{\sigma}}$  are available, whereas the plastic part requires an incremental-iterative solution procedure at material integration

point level, following a fully implicit (backward Euler) integration scheme of the rate form of the constitutive equations. Newton's method is used for the resolution of the resulting nonlinear constitutive system of equations. As thoroughly illustrated in Grassl and Jirásek (2006a), and summarised here as reference in Figure 3.2, the effective stress evaluation is based on the standard division into elastic predictor and plastic corrector, where isotropy of the plastic potential  $g_p$  along with its independence of Lode's angle  $\bar{\theta}$  allows for a compact (rank 4) form of the residual system:

$$\begin{aligned}\bar{\sigma}_V &= \bar{\sigma}_V^{tr} - K \Delta\lambda m_V(\bar{\sigma}, \kappa_p) \\ \bar{\rho} &= \bar{\rho}^{tr} - 2G \Delta\lambda m_D(\bar{\sigma}, \kappa_p) \\ \kappa_p &= \kappa_p^{(n)} + \Delta\lambda k_p(\bar{\sigma}, \kappa_p) \\ f_p(\bar{\sigma}, \kappa_p) &= 0\end{aligned}\tag{3.31}$$

as  $\bar{\theta} = \bar{\theta}^{tr}$  can be computed and stored from the elastic trial state  $\bar{\sigma}^{tr}$  throughout the whole stress-return. In equation (3.31), all field variables refer to incremental step  $(n+1)$ , whereby this index has been dropped for clarity,  $m_V = \mathbf{m} : \boldsymbol{\delta}$  and  $m_D = \|\mathbf{m} - m_V \boldsymbol{\delta} / 3\|$  are the volumetric and deviatoric invariants of the flow direction,  $K$  and  $G$  are the elastic bulk and shear moduli, and  $\lambda$  is the plastic multiplier. The output of the plastic part at the end of each incremental step is consequently the updated set of effective stresses  $\bar{\sigma}$ , plastic strains  $\boldsymbol{\varepsilon}_p$ , internal plastic hardening variable  $\kappa_p$  and plastic multiplier  $\lambda$  (Figure 3.2). Similarly, the output of the damage part includes the updated set of damage parameter  $\omega$ , internal damage-driving variable  $\kappa_d$  and nominal stresses  $\boldsymbol{\sigma}$  in the case of isotropic damage. For the generalised anisotropic version, the output consists of the damage tensor  $\boldsymbol{\omega}$ , its trace  $\kappa_d$  and nominal stresses  $\boldsymbol{\sigma}$ .

As shown in Figure 3.1, the meridians contained on any meridian plane intersect the hydrostatic axis at 2 points called apexes. Upon hardening completion, the initially closed elastic envelope becomes open from the compressive side, whereas the tensile apex barely moves along the hydrostatic axis until it gets fixed at a volumetric stress  $\bar{\sigma}_{V,apex}^t = \bar{f}_c / m_0$ . For the treatment of these apexes no cut-off functions are defined. Instead, different types of stress-return are formulated whilst maintaining the formal structure and the rank of the system of equations (rank 4).

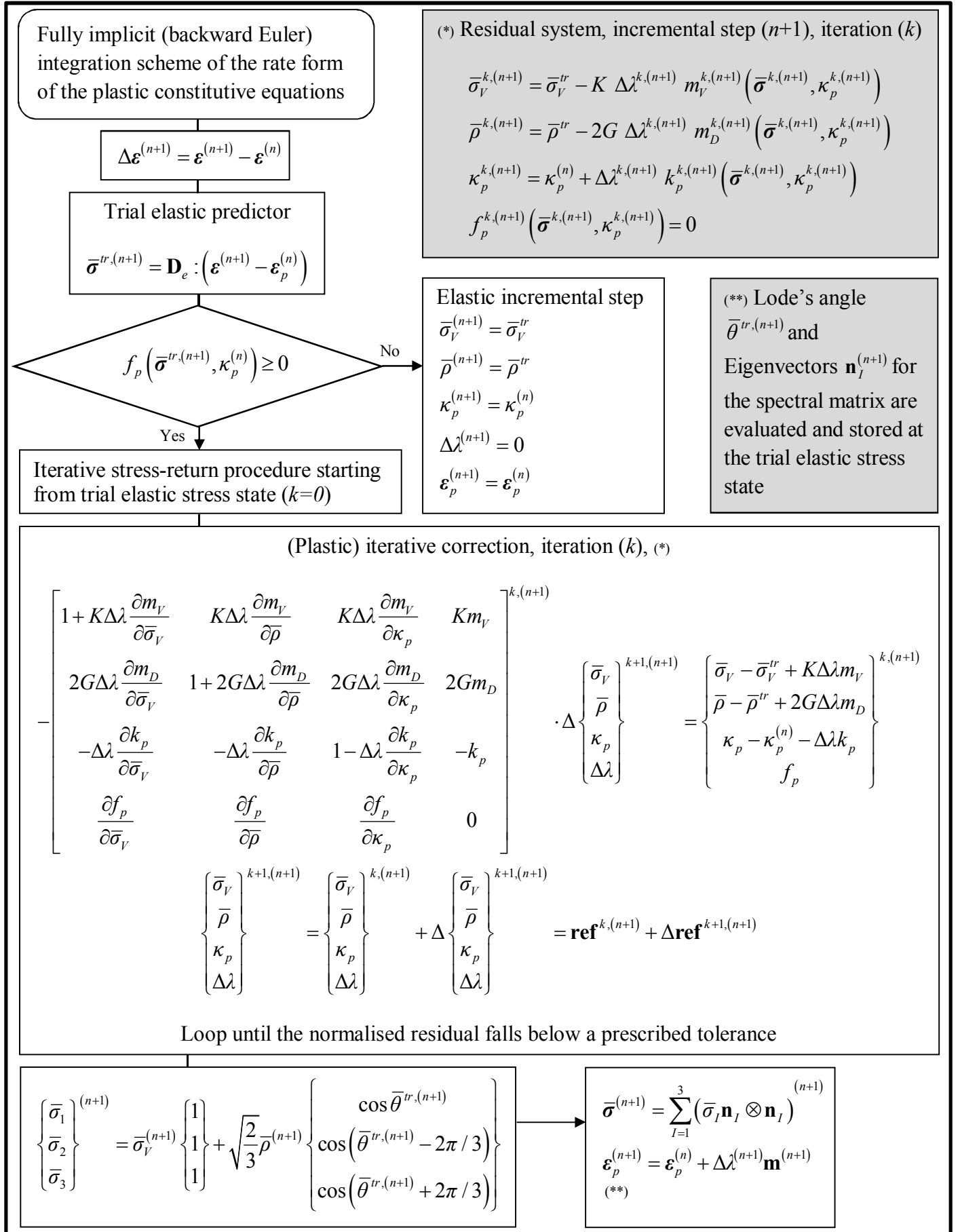


Figure 3.2: Flowchart of the plastic standard iterative stress-return procedure

As the gradient of the plastic potential  $\mathbf{m}$  is not uniquely defined at the apexes, there is an admissible set of sub-gradients  $\partial\mathbf{m}$  enclosed in (complementary) cones defined initially in the strain space and then converted to their stress equivalents. The fact that the complementary surfaces are cones is a direct consequence of the plastic potential being a set of revolution surfaces.

Whilst hardening is ongoing, the vertex and slope of such cones at the end of the step are unknown, whereas upon completion of hardening there is only a tensile cone, fixed in the stress space along with the failure surface of Menétrey and Willam (3.10). Hence, by tracking the development of the hardening process and a simple geometrical assessment, checking if the trial stress state is inside an initial cone (as defined at the beginning of the incremental step), three types of stress-return can be distinguished depending of the output of this *a priori* check:

- Iterative apex return: hardening is ongoing ( $0 < \kappa_p < 1$ ) and the stress-return leads to an apex of unknown volumetric coordinate.
- Direct apex return: hardening is complete ( $\kappa_p \geq 1$ ), the apex is fixed and hence the stress-return does not need to iterate.
- Standard return: irrespective of the hardening state, the stress-return leads to an unknown point on the smooth part of the surface. Further provisions may be taken, as explained in Section 3.3.1.

The flowchart distinguishing all return types is depicted in Figure 3.3. Formally, the *a priori* check compares – in the meridian plane defined by  $\bar{\theta}^{tr}$  – the slope of the line passing through the apex in consideration and the elastic trial stress point with the slope of the corresponding complementary cone in stress space:

$$\frac{K}{2G} \left( \frac{\partial \mathbf{g}_p}{\partial \bar{\sigma}_V} \right)_{apex}^{(n)} \longleftrightarrow \left( \frac{\bar{\sigma}_V^{tr} - \bar{\sigma}_{V,apex}^{(n)}}{\bar{\rho}^{tr}} \right) \quad (3.32)$$

with:

$$\left. \frac{\partial \mathbf{g}_p}{\partial \bar{\sigma}_V} \right|_{apex}^{(n)} = (1 - q_h)^2 \frac{4}{\bar{f}_c} \left( \frac{\bar{\sigma}_{V,apex}^{(n)}}{\bar{f}_c} \right)^3 + \frac{q_h^2}{\bar{f}_c} A_g \exp \left( \frac{\bar{\sigma}_{V,apex}^{(n)} - \bar{f}_t}{B_g \bar{f}_c} \right) \quad (3.33)$$

$$\left. \frac{\partial g_p}{\partial \bar{\rho}} \right|_{apex}^{(n)} = (1 - q_h)^2 \frac{4}{\sqrt{6} \bar{f}_c} \left( \frac{\bar{\sigma}_{V,apex}^{(n)}}{\bar{f}_c} \right)^3 + \frac{\sqrt{6}}{\bar{f}_c} (1 - q_h) \left( \frac{\bar{\sigma}_{V,apex}^{(n)}}{\bar{f}_c} \right)^2 + q_h^2 \frac{m_0}{\sqrt{6} \bar{f}_c} \quad (3.34)$$

and  $\bar{\sigma}_{V,apex}^{(n)}$  being the appropriate solution of the quartic equation:

$$(1 - q_h)^2 \left( \frac{\bar{\sigma}_V}{\bar{f}_c} \right)^4 + m_0 q_h^2 \left( \frac{\bar{\sigma}_V}{\bar{f}_c} \right) - q_h^2 = 0 \quad (3.35)$$

evaluated at the previous incremental step  $(n)$ , as can be easily derived from (3.5) by substituting  $\bar{\rho} = 0$ .

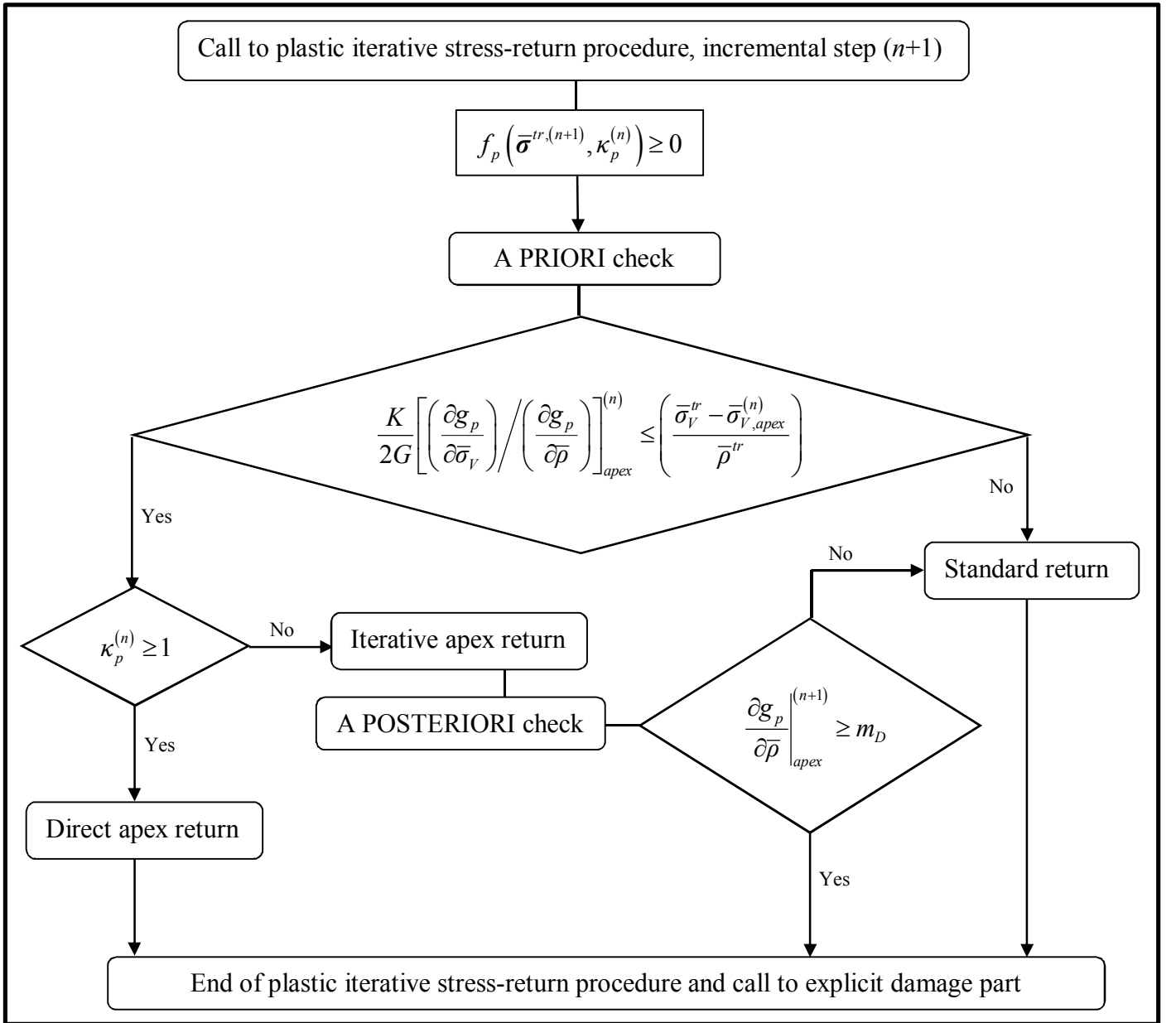


Figure 3.3: Iterative stress-return types depending on check evaluation

For the tensile case, a simple bisection scheme suffices to establish  $\bar{\sigma}_{V,apex}^{t,(n)}$  from (3.35). For the compressive case, the consideration that  $q_h^2$  is progressively negligible as compared to  $m_0 q_h^2 \left( \frac{\bar{\sigma}_V}{\bar{f}_c} \right)$  leads to the following iterative estimation of  $\bar{\sigma}_{V,apex}^{c,(n)}$ :

$$\bar{\sigma}_{V,apex}^{c,(n,k+1)} = -\bar{f}_c \left( \frac{q_h^2 - m_0 q_h^2 \left( \frac{\bar{\sigma}_{V,apex}^{c,(n,k)}}{\bar{f}_c} \right)}{(1-q_h)^2} \right)^{\frac{1}{4}} \quad (3.36)$$

$$\bar{\sigma}_{V,apex}^{c,(n,0)} = -\bar{f}_c \left( \frac{m_0 q_h^2}{(1-q_h)^2} \right)^{\frac{1}{3}}$$

with its exact absolute value as an upper bound, so that  $k = 0, 1, 2, \dots$  until a certain tolerance is satisfied.

Should a direct apex return apply, then the *a priori* check is both necessary and sufficient, with the following explicit expressions for the update of state variables:

$$m_V = \frac{A_g}{\bar{f}_c} \exp \left( \frac{\left( \frac{\bar{f}_c - \bar{f}_t}{m_0} \right) \frac{3}{B_g \bar{f}_c}} \right) \quad (3.37)$$

$$m_D = \frac{\bar{\rho}^{tr} K m_V}{2G \left( \frac{\bar{\sigma}_V^{tr} - \bar{f}_c}{m_0} \right)} \quad (3.38)$$

$$\Delta\lambda = \frac{\bar{\sigma}_V^{tr} - \bar{f}_c}{K m_V} \quad (3.39)$$

The case of iterative apex return, however, requires an additional *a posteriori* check:

$$\left. \frac{\partial g_p}{\partial \bar{\rho}} \right|_{apex}^{(n+1)} \xleftrightarrow{?} m_D \quad (3.40)$$

since the complementary cones may have shifted in the stress space to a sufficient extent not to enclose the trial state in their updated position. If the *a posteriori* check is not satisfied, it is

necessary to reset the state variables to their initial values and proceed with the standard return.

Considering the residual equation for deviatoric radius (3.31), if  $\bar{\rho}$  is enforced to be zero, the deviatoric invariant of the flow direction  $m_D$  can be considered as an independent variable (the deviatoric component of the non-unique sub-gradient  $\partial \mathbf{m}$ ) instead of a function of the updated state variables:

$$\begin{aligned} \bar{\sigma}_V - \bar{\sigma}_V^{tr} + K \Delta\lambda m_V(\bar{\sigma}_V, \kappa_p) &= 0 \\ -\bar{\rho}^{tr} + 2G \Delta\lambda m_D &= 0 \\ \kappa_p - \kappa_p^{(n)} - \Delta\lambda k_p(\bar{\sigma}_V, m_D, \kappa_p) &= 0 \\ f_p(\bar{\sigma}_V, \kappa_p) &= 0 \end{aligned} \quad (3.41)$$

with  $f_p$ ,  $m_V$  and  $k_p$  particularised to  $\bar{\rho} = 0$ . The resulting system (3.41) is the iterative apex return particularisation of the standard return case (Figure 3.2). By making the corresponding adjustments in the related terms of the Jacobian matrix, the iterative apex return may then make use of a similar rank 4 system of equations to the standard return case when entering the Newton scheme for resolution:

$$\mathbf{Jac} = \begin{bmatrix} 1 + K\Delta\lambda \frac{\partial m_V}{\partial \bar{\sigma}_V} & 0 & K\Delta\lambda \frac{\partial m_V}{\partial \kappa_p} & Km_V \\ 0 & 2G\Delta\lambda & 0 & 2Gm_D \\ -\Delta\lambda \frac{\partial k_p}{\partial \bar{\sigma}_V} & -\Delta\lambda \frac{\partial k_p}{\partial m_D} & 1 - \Delta\lambda \frac{\partial k_p}{\partial \kappa_p} & -k_p \\ \frac{\partial f_p}{\partial \bar{\sigma}_V} & 0 & \frac{\partial f_p}{\partial \kappa_p} & 0 \end{bmatrix} \quad (3.42)$$

In order to avoid initial Jacobian singularity when starting the iterative solution procedure from the trial elastic state, implying  $\Delta\lambda = 0$  and a null second column in **Jac**, a further division in 2 stages is enforced in the stress-return, i.e. a first stage with a direct apex stress-return followed by an iterative stage along the hydrostatic axis. For stage 1, if the stress-return leads to the tensile apex, equations (3.37) to (3.39) are used. Should the stress-return lead to the compressive apex, then stage 1 requires equation (3.39) to be adapted to:

$$\Delta\lambda = \frac{|\sigma_V^{tr} - \sigma_{V,apex}^{(n)}|}{K |m_V|} \quad (3.43)$$

with:

$$m_V = \left(1 - q_h^{(n)}\right)^2 \frac{4}{\bar{f}_c} \left(\frac{\bar{\sigma}_V}{\bar{f}_c}\right)^3 + \frac{(q_h^{(n)})^2}{\bar{f}_c} A_g \left(\frac{\bar{\sigma}_V - \frac{\bar{f}_t}{3}}{B_g \bar{f}_c}\right) \quad (3.44)$$

That is, the iterative stage along the hydrostatic axis starts from the final apex  $\bar{\sigma}_{V,apex}^t = \frac{\bar{f}_c}{m_0}$  in the tensile domain whereas in the compressive domain it starts from the apex of the previous iterative step  $\sigma_{V,apex}^{c,(n)}$ .

For any apex return, the resulting Jacobian is directly used for the calculation of the algorithmic elastic-plastic-damage stiffness  $\Theta_{EPD}$  (see Section 3.4). Once the stress-return evaluation has been completed, the update of the isotropic damage related state variables is direct, as schematically shown in Figure 3.4.

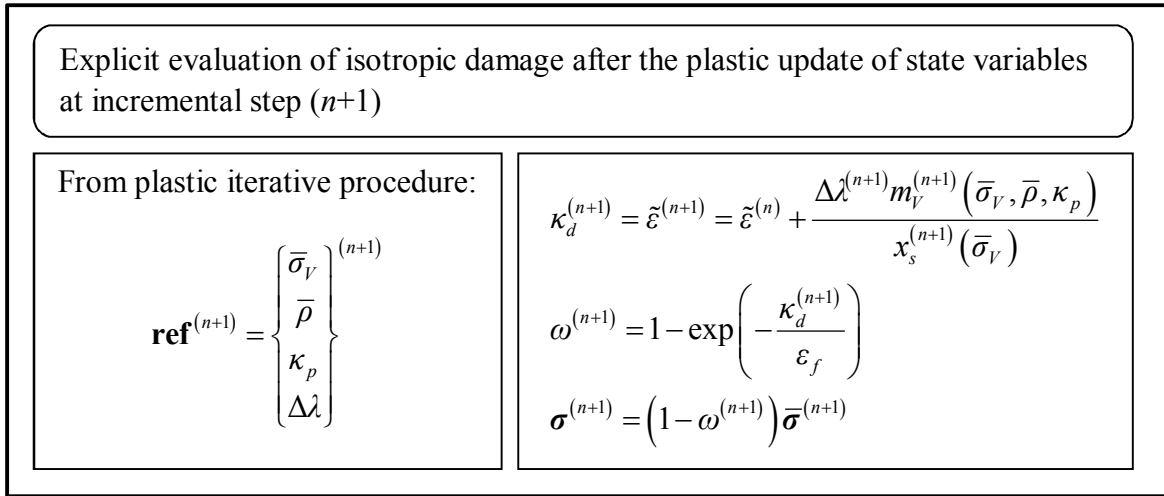


Figure 3.4: Update of isotropic damage variables following plastic stress-return

Similarly, the case of anisotropic damage also keeps the explicit character in the evaluation of the updated variables, although the internal strain-like variable changes its meaning. By enforcing the consistency condition  $\dot{f}_d = 0$  on (3.26) and substituting (3.27), the following rate relation between damage and total strain tensors is obtained:

$$\dot{\omega} = \left( \frac{\mathbf{g}_d' \boldsymbol{\varepsilon}_p^2 \otimes \boldsymbol{\eta}}{\boldsymbol{\delta} : \boldsymbol{\varepsilon}_p^2} \right) : \dot{\boldsymbol{\varepsilon}} = \mathbf{M}_\omega : \dot{\boldsymbol{\varepsilon}} \quad (3.45)$$

The sign  $\otimes$  stands for direct (or outer) product, and the remaining components are defined as:

$$\mathbf{g}_d' = \frac{d\mathbf{g}_d}{d\tilde{\varepsilon}} \quad (3.46)$$

$$\boldsymbol{\eta} = \frac{\partial \tilde{\varepsilon}}{\partial \boldsymbol{\varepsilon}} \quad (3.47)$$

Hence, (3.45)-(3.47) along with (3.28)-(3.29) allow for the incremental update of the relevant variables as shown in Figure 3.5.

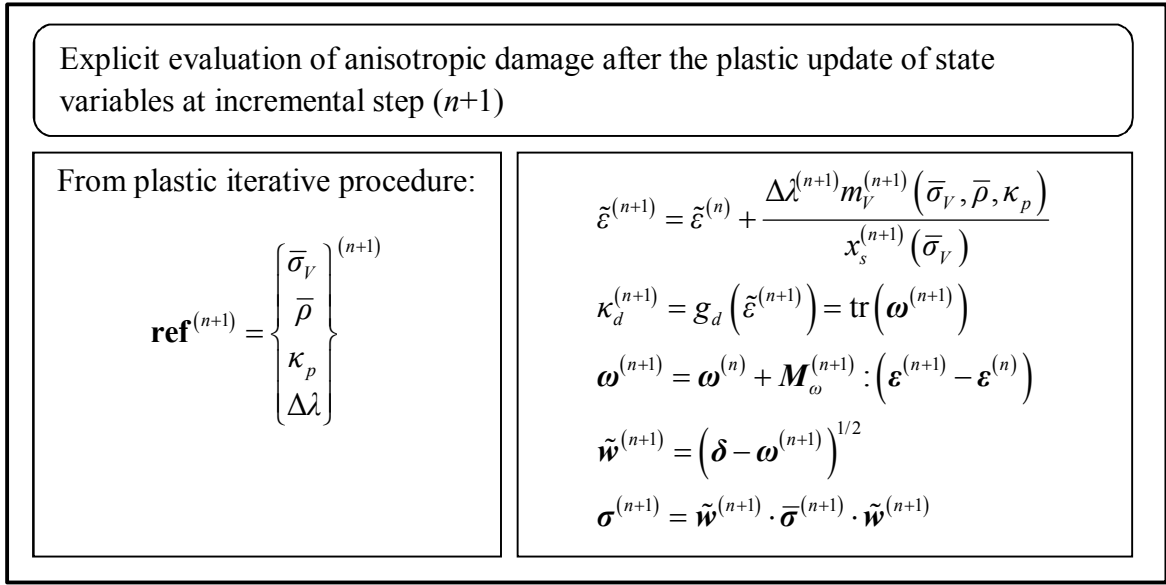


Figure 3.5: Update of anisotropic damage variables following plastic stress-return

### 3.3.1 Further computational issues under standard stress-return

Although the algorithmic architecture as schematically represented in Figures 3.2, 3.3 and 3.4 or 3.5 allows for a systematic and effective treatment of all possible stress-return types based on geometric arguments, there are issues of computational nature affecting the standard iterative return procedure. These are mainly two: the potential singularity of the Jacobian and the proneness to *overshooting* from certain regions of the effective stress space during stress-return. Either of them, or their combination, can seriously hinder convergence (by dropping the convergence rate or even by inducing divergence) or mislead the procedure to converge to inadmissible values. Consequently, the novel remedies described hereafter to address these issues contribute significantly to the algorithmic robustness, as is shown by means of a numerical test.

### 3.3.1.1 Initial Jacobian singularity and system reduction

The Jacobian matrix associated to the standard stress-return along a fixed meridian plane:

$$\mathbf{Jac} = \begin{bmatrix} 1 + K\Delta\lambda \frac{\partial m_V}{\partial \bar{\sigma}_V} & K\Delta\lambda \frac{\partial m_V}{\partial \bar{\rho}} & K\Delta\lambda \frac{\partial m_V}{\partial \kappa_p} & Km_V \\ 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\sigma}_V} & 1 + 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\rho}} & 2G\Delta\lambda \frac{\partial m_D}{\partial \kappa_p} & 2Gm_D \\ -\Delta\lambda \frac{\partial k_p}{\partial \bar{\sigma}_V} & -\Delta\lambda \frac{\partial k_p}{\partial \bar{\rho}} & 1 - \Delta\lambda \frac{\partial k_p}{\partial \kappa_p} & -k_p \\ \frac{\partial f_p}{\partial \bar{\sigma}_V} & \frac{\partial f_p}{\partial \bar{\rho}} & \frac{\partial f_p}{\partial \kappa_p} & 0 \end{bmatrix} \quad (3.48)$$

is sensitive to singularity around an initial trial elastic stress state at any stage during the hardening process, as shown below:

$$\mathbf{Jac}_0 = \begin{bmatrix} 1 & 0 & 0 & Km_V \\ 0 & 1 & 0 & 2Gm_D \\ 0 & 0 & 1 & -k_p \\ \frac{\partial f_p}{\partial \bar{\sigma}_V} & \frac{\partial f_p}{\partial \bar{\rho}} & \frac{\partial f_p}{\partial \kappa_p} & 0 \end{bmatrix} \quad (3.49)$$

$\begin{matrix} \bar{\sigma}_V = \bar{\sigma}_V^{tr} \\ \bar{\rho} = \bar{\rho}^{tr} \\ \Delta\lambda = 0 \\ 0 \leq \kappa_p^{(n)} < 1 \end{matrix}$

$$\det(\mathbf{Jac}_0) = \frac{\partial f_p}{\partial \bar{\sigma}_V} Km_V + \frac{\partial f_p}{\partial \bar{\rho}} 2Gm_D - \frac{\partial f_p}{\partial \kappa_p} k_p \quad (3.50)$$

The determinant of the Jacobian in (3.50) can become zero for a certain admissible range of trial volumetric stresses and deviatoric radii, whereby it becomes apparent that the increments of the state variables are perpendicular to the gradient of the yield function in the  $(\bar{\sigma}_V, \bar{\rho}, \kappa_p)$  space. Figure 3.6 further demonstrates this by showing the shape of the determinant of the initial Jacobian for  $\kappa_p^{(n)} = 0$  in the  $(\bar{\sigma}_V^{tr}, \bar{\rho}^{tr})$  compressive meridian plane  $\left(\bar{\theta}^{tr} = \frac{\pi}{3}\right)$ , for a given set of material parameters within the typical range for concrete.

The intersection of the surface depicted in Figure 3.6 with the zero-determinant plane forms a contour line, the evolution of which is shown in Figure 3.7 for various initial values of the hardening internal variable  $\kappa_p^{(n)}$ , together with the corresponding elastic envelope (i.e. initial yield surface) and final meridian.

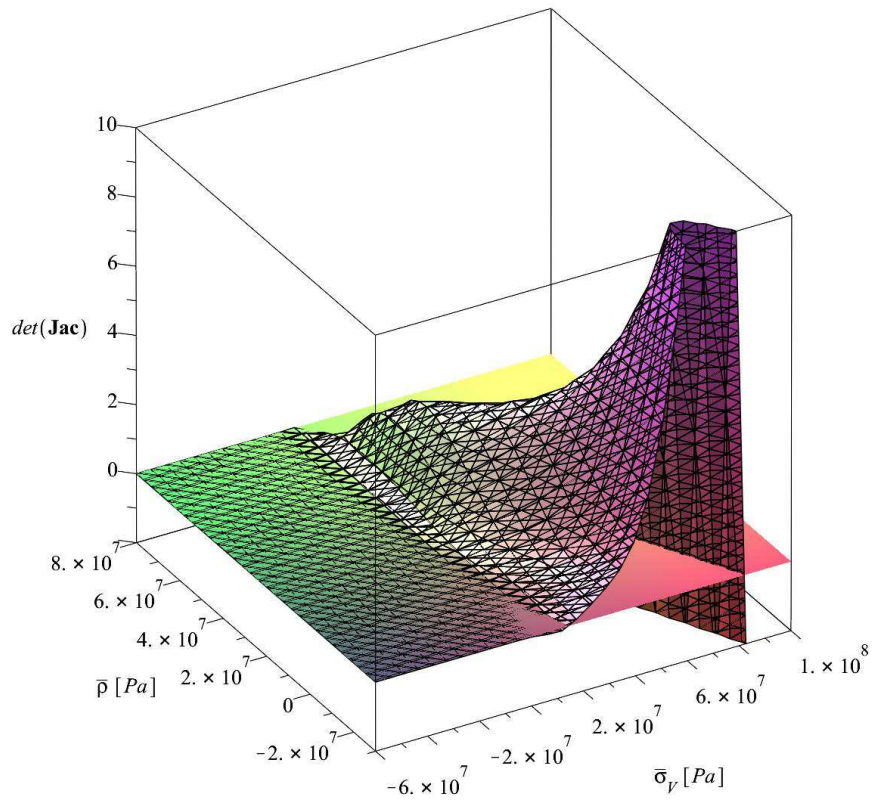
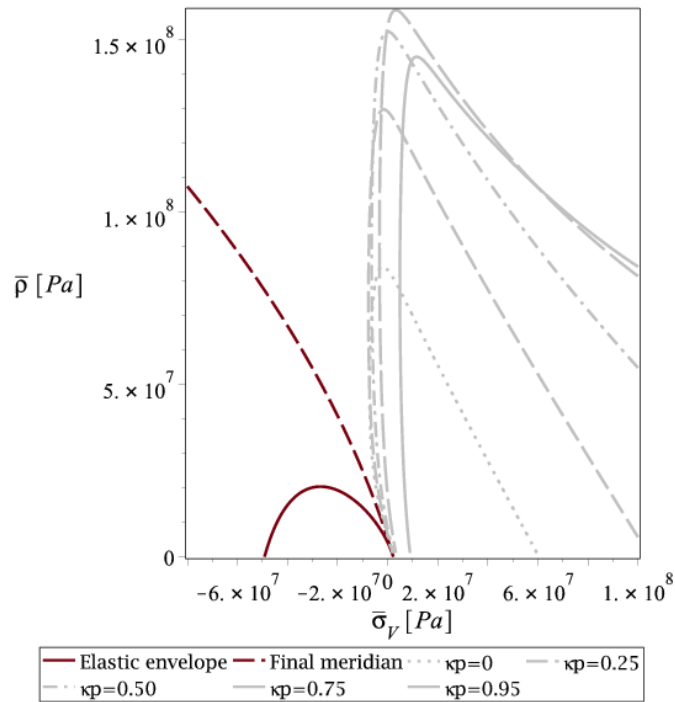


Figure 3.6: Determinant of the initial Jacobian and its zero plane


 Figure 3.7: Evolution of contour  $\det(\mathbf{Jac}_0) = 0$  for  $0 \leq \kappa_p^{(n)} \leq 0.95$  with  $\bar{\theta}^{tr} = \frac{\pi}{3}$

The contour of singularity of the initial Jacobian encloses a region where the sign of the determinant of  $\mathbf{Jac}_0$  is opposite to the rest of the meridian plane, and hence it can no longer be guaranteed that the iterative correction from the Newton scheme has a reducing character on the convergence measure, i.e.  $\Delta \mathbf{ref}$  in Figure 3.2 may not be a descent direction. Furthermore, the contour itself evolves along a significant region of admissible effective stress states, getting particularly close to the final meridian in the vicinity of the tensile apex, and thus potentially posing great convergence issues during the hardening process, as the contour shifts towards (positive) infinite  $\bar{\sigma}_v$  as  $\kappa_p \rightarrow 1$  (Figure 3.9).

In order to overcome the aforementioned drawback, it is illustrative to investigate the shape of the boundary separating trial stress points returning to the Men  trety-Willam surface (3.10) from those returning to yield surfaces in the process of hardening in a single incremental step, i.e. the locus marking single-step stress-returns with  $\Delta \kappa_p \geq 1$ . Such locus can be derived following a basic iterative procedure, and is shown in Figure 3.8 both for the compressive  $\left(\bar{\theta}^{tr} = \frac{\pi}{3}\right)$  and the tensile  $\left(\bar{\theta}^{tr} = 0\right)$  meridian planes. As can be noticed when comparing Figures 3.7 and 3.8, the region bounded by the singularity contours of the determinant of the initial Jacobian is mostly contained at the side of the locus where hardening has finished.

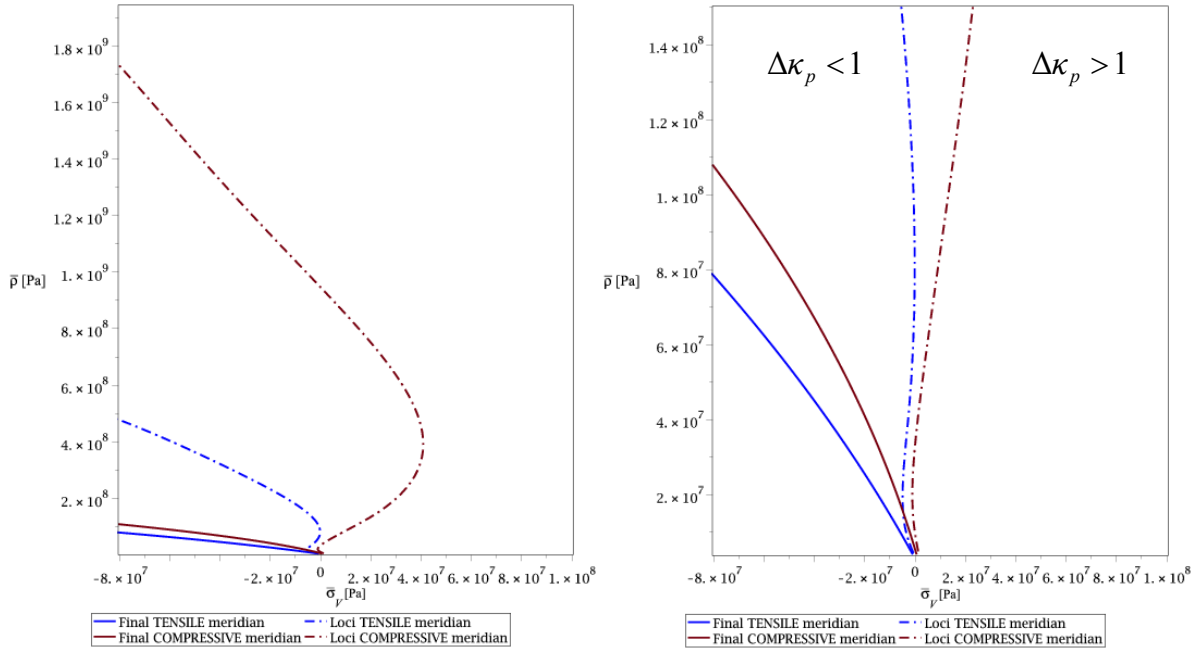


Figure 3.8: Loci of trial stress points returning to the final meridians in a single-step stress-return along the compressive and tensile meridian plane

In view of this feature, and since the singularity contours of the initial Jacobian are located in the softening domain, it is proposed to subject the standard return to a further reduction if the trial elastic stress state lies outside of the Men  trety-Willam surface (3.10), formally following a similar reasoning as in the case of an iterative apex stress-return. In such a case, it is assumed that perfect plasticity is reached at the end of the incremental step, which allows for the decoupling of  $\kappa_p$  from the system of equations (decoupling of (3.31) from the rest of the system), since the stress-return leads to a surface fixed in stress space, and thereby reducing its rank to 3. This implies enforcing the normalised hardening variable to be  $q_h = 1$  in the 3 remaining equations of the system given by (3.31).

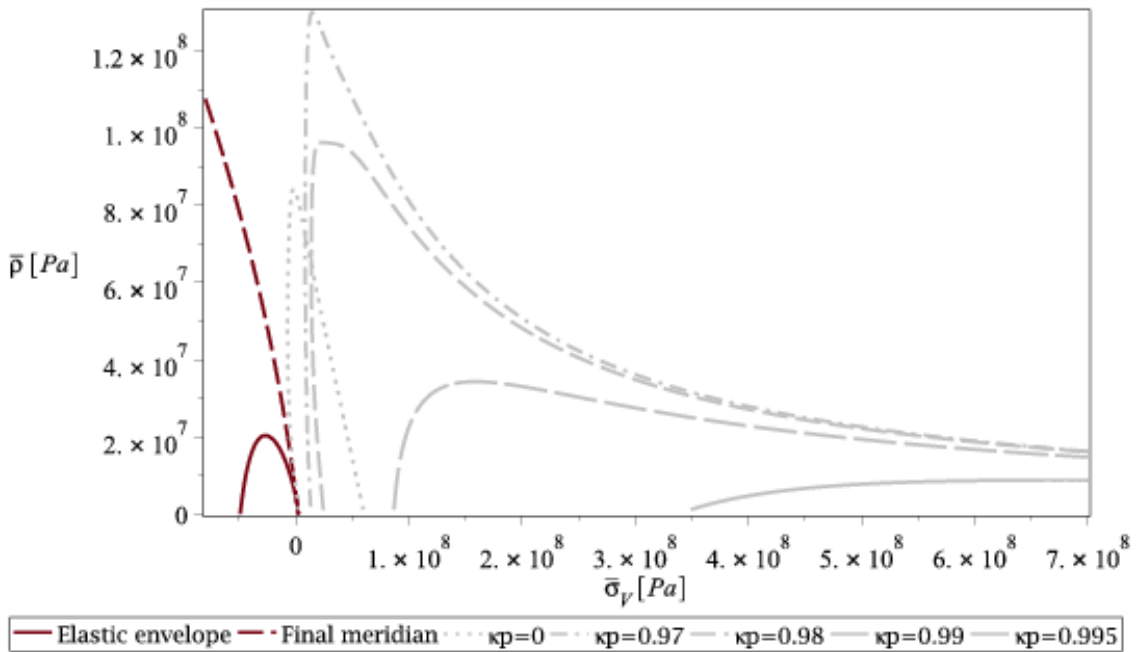


Figure 3.9: Evolution of contour  $\det(\mathbf{Jac}_0) = 0$  on the compressive meridian plane  $\bar{\theta}^{tr} = \frac{\pi}{3}$

The decoupled state variable  $\kappa_p$  can be calculated *a posteriori*, via (3.31), further resorting to the original rank 4 formulation if necessary should  $\kappa_p < 1$  follow from this, shifting the initial state from the trial elastic coordinates to the previously obtained ones on the failure surface.

If  $\kappa_p^{(n)} \geq 1$ , the reduced system formulation keeps its validity throughout, and  $\kappa_p \geq \kappa_p^{(n)}$  as  $\Delta\lambda \geq 0$  and  $k_p > 0$ . Moreover, when  $\kappa_p^{(n)} < 1$ , if the trial elastic stress state lies somewhere between the elastic envelope and the Men  trety-Willam surface, it is ensured that the singularity contour will not be crossed during stress-return, and hence the standard rank 4 formulation is applicable to obtain the updated values of all state variables at once.

In general, the term enabling the possibility of the full initial Jacobian becoming singular during hardening is  $\mathbf{Jac}_0(3,4) = -k_p$ , as can be easily verified by inspecting (3.49), since

$\frac{\partial f_p}{\partial \kappa_p} = 0$  once hardening has reached completion. Decoupling  $\kappa_p$  as described above allows

for expressing the reduced Jacobian associated to the standard stress-return as:

$$\mathbf{Jac} = \begin{bmatrix} 1 + K\Delta\lambda \frac{\partial m_V}{\partial \bar{\sigma}_V} & K\Delta\lambda \frac{\partial m_V}{\partial \bar{\rho}} & Km_V \\ 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\sigma}_V} & 1 + 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\rho}} & 2Gm_D \\ \frac{\partial f_p}{\partial \bar{\sigma}_V} & \frac{\partial f_p}{\partial \bar{\rho}} & 0 \end{bmatrix}_{q_h=1} = \begin{bmatrix} 1 + K\Delta\lambda \frac{\partial m_V}{\partial \bar{\sigma}_V} & 0 & Km_V \\ 0 & 1 + 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\rho}} & 2Gm_D \\ \frac{\partial f_p}{\partial \bar{\sigma}_V} & \frac{\partial f_p}{\partial \bar{\rho}} & 0 \end{bmatrix}_{q_h=1} \quad (3.51)$$

since  $\frac{\partial m_V}{\partial \bar{\rho}} = 0$  and  $\frac{\partial m_D}{\partial \bar{\sigma}_V} = 0$  under the assumption  $q_h = 1$ . For the case of the initial Jacobian,

equation (3.51) further simplifies to:

$$\mathbf{Jac}_0 = \begin{bmatrix} 1 & 0 & Km_V \\ 0 & 1 & 2Gm_D \\ \frac{\partial f_p}{\partial \bar{\sigma}_V} & \frac{\partial f_p}{\partial \bar{\rho}} & 0 \end{bmatrix}_{\substack{\bar{\sigma}_V = \bar{\sigma}_V^{tr} \\ \bar{\rho} = \bar{\rho}^{tr} \\ \Delta\lambda = 0 \\ q_h = 1}} \quad (3.52)$$

Similar to (3.50) arising from the singularity conditions of the full initial Jacobian (3.49), the singularity of the reduced initial Jacobian (3.52) leads to the following condition:

$$Km_V \frac{\partial f_p}{\partial \bar{\sigma}_V} + 2Gm_D \frac{\partial f_p}{\partial \bar{\rho}} = 0 \quad (3.53)$$

where all intervening functions are assessed as:

$$\begin{aligned}
 m_V &= \frac{A_g}{f_c} \exp\left(\frac{\bar{\sigma}_V - \bar{f}_t/3}{B_g \bar{f}_c}\right) > 0 \quad \forall \bar{\sigma}_V \\
 m_D &= \frac{1}{\bar{\rho}} \left( \frac{3\bar{\rho}}{f_c^2} + \frac{m_0}{\sqrt{6} f_c} \right) \|\mathbf{J}_{2,\bar{\sigma}}\| > 0 \quad \forall \bar{\rho} > 0 \\
 \frac{\partial f_p}{\partial \bar{\sigma}_V} &= \frac{m_0}{f_c} = \text{constant} > 0 \\
 \frac{\partial f_p}{\partial \bar{\rho}} &= \frac{3\bar{\rho}}{f_c^2} + \frac{m_0}{f_c} \frac{r(e, \bar{\theta}^{tr})}{\sqrt{6}} > 0 \quad \forall \bar{\rho} > 0
 \end{aligned} \tag{3.54}$$

with  $\mathbf{J}_{2,\bar{\sigma}} = \frac{\partial \mathbf{J}_2}{\partial \bar{\sigma}}$  and  $r$  being the Willam and Warnke function as defined in (3.6).

Consequently, condition (3.53) cannot be fulfilled under trial elastic conditions, as definitions (3.2) and (3.4) guarantee that the trial deviatoric radius remains positive, and hence regularity of the reduced initial Jacobian is ensured. This can be further demonstrated by inspecting the shape of its determinant in the compressive meridian plane, shown in Figure 3.10, and comparing it to its full formulation counterpart shown in Figure 3.6.

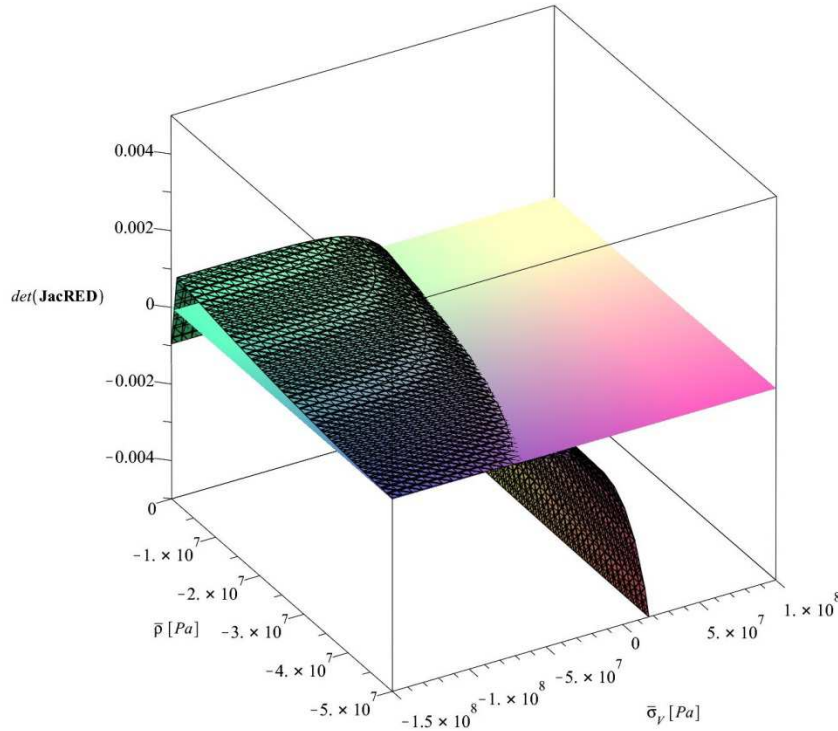


Figure 3.10: Determinant of the reduced initial Jacobian and its zero plane

The contour of singularity falls entirely into the inadmissible stress domain of negative deviatoric radii, as can be seen in Figure 3.11:

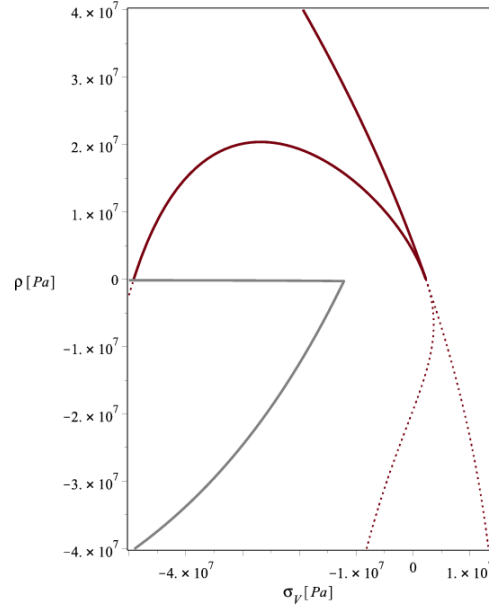


Figure 3.11: Contour  $\det(\mathbf{Jac}_0) = 0$  (grey) for  $\Delta\lambda = 0$  on the compressive meridian plane

$$\bar{\theta}^{ir} = \frac{\pi}{3} \text{ (meridians in red, solid in the admissible domain and dotted otherwise)}$$

Reduced Jacobian regularity at initial trial conditions aside, its potential singularity and the associated convergence issues are susceptible to occur in subsequent iterative states within the same incremental step, especially when the stress-return aims at the tensile domain of the yield surface where nonlinearity is more pronounced. To illustrate this, Figure 3.12 shows the initial evolution of the singularity contour with the plastic multiplier, starting from  $\Delta\lambda = 0$ .

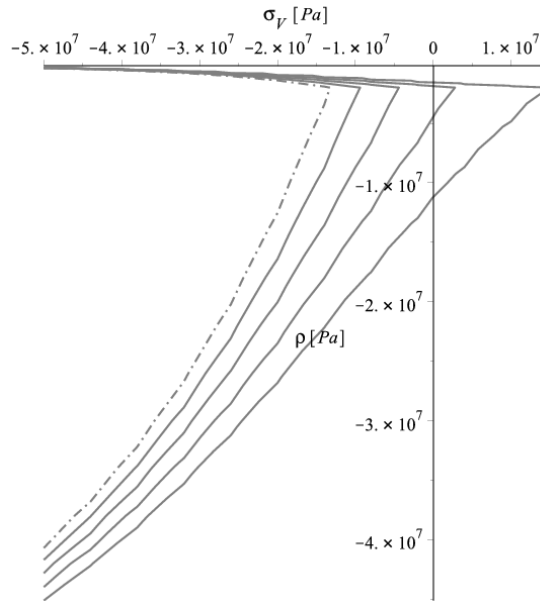


Figure 3.12: Evolution of contour  $\det(\mathbf{Jac}) = 0$  under reduced formulation for  $\Delta\lambda = 0$  (dashed) and further increasing  $\Delta\lambda > 0$  (solid) in the compressive meridian plane

In iterative states with  $\Delta\lambda \neq 0$ , the singularity contour under the reduced formulation shifts along the direction of positive  $\bar{\sigma}_V$ , thereby entering a region of the meridian plane which, though inadmissible ( $\bar{\sigma}_V > 0, \bar{\rho} < 0$ ), is prone to contain iterative solutions as the iterative procedure may incur *overshooting*. This is particularly the case when the standard stress-return is meant to reach the smooth area of the yield surface in the vicinity of the tensile apex. Formally, the generalisation of condition (3.53) representing the singularity of the reduced Jacobian at intermediate iterative states follows from enforcing a null determinant of the Jacobian in (3.51):

$$Km_V \frac{\partial f_p}{\partial \bar{\sigma}_V} \left( 1 + 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\rho}} \right) + 2Gm_D \frac{\partial f_p}{\partial \bar{\rho}} \left( 1 + K\Delta\lambda \frac{\partial m_V}{\partial \bar{\sigma}_V} \right) = 0 \quad (3.55)$$

where equation (3.55) can only be satisfied for negative deviatoric radii. In order to ensure Jacobian regularity throughout the whole stress-return process, and to overcome the aforementioned convergence difficulties arising from *overshooting*, a basic line search technique is proposed and discussed in the following section.

### 3.3.1.2 Line search/Damping of Newton scheme

Along with trust-region methods, line search is one of the most widespread global convergence strategies. A detailed description of its properties and requirements can be found in (Deuffhard, 2004; Crisfield, 1982), whereas in the present section only the basic features of such method are presented and utilised.

Generally, within the framework of a full-Newton iterative scheme, application of a line search strategy implies accepting the corrective direction given by the Newton scheme whilst resorting to an a posteriori modulation of the corrective step-length, via a damping factor  $\alpha$ . Hence, the expression for the iterative correction in Figure 3.2 is generalised as:

$$\mathbf{ref}^{k+1,(n+1)} = \mathbf{ref}^{k,(n+1)} + \alpha^{k+1,(n+1)} \cdot \Delta \mathbf{ref}^{k+1,(n+1)} \quad (3.56)$$

subject to  $\alpha^{k+1,(n+1)} \in ]0,1]$ , with:

$$\mathbf{ref}^{k,(n+1)} = \begin{Bmatrix} \bar{\sigma}_V \\ \bar{\rho} \\ \Delta\lambda \end{Bmatrix}^{k,(n+1)} \quad (3.57)$$

under the current reduced formulation. An exact line search would obtain  $\alpha^{k+1,(n+1)}$  as the solution of the global minimization problem of the univariate function:

$$H\left(\alpha^{k,(n+1)}\right)=\left\|\mathbf{r}\left(\mathbf{ref}^{k,(n+1)}+\alpha^{k+1,(n+1)}\cdot\Delta\mathbf{ref}^{k+1,(n+1)}\right)\right\| \quad (3.58)$$

where  $\mathbf{r}$  is the residual vector of the reduced system of equations (Figure 3.2):

$$\mathbf{r}^{k,(n+1)}=\left\{\begin{matrix} \mathbf{r}_\sigma \\ \mathbf{r}_\rho \\ \mathbf{r}_f \end{matrix}\right\}^{k,(n+1)}=\left\{\begin{matrix} \bar{\sigma}_V^{k,(n+1)}-\bar{\sigma}_V^{tr}+K\Delta\lambda^{k,(n+1)}m_V^{k,(n+1)} \\ \bar{\rho}^{k,(n+1)}-\bar{\rho}^{tr}+2G\Delta\lambda^{k,(n+1)}m_D^{k,(n+1)} \\ f_p^{k,(n+1)} \end{matrix}\right\} \quad (3.59)$$

However, exact line search is typically too costly and therefore inexact line search strategies are preferred, where acceptable reductions in  $\|\mathbf{r}\|$  are achieved by means of satisfying certain criteria, e.g. the Wolfe conditions (Deuffhard, 2004). In the present case, the measure of damping in the iterative corrective step-length is not based on optimization arguments but postulated as an intuitive geometric constraint in the effective stress space, and the validity of such strategy is checked qualitatively *a posteriori*. This has been considered appropriate since the original reason for introducing damping is not that of minimising  $\|\mathbf{r}\|$  for a given correction but avoiding the singularity contours of Figure 3.12 during stress-return under the reduced formulation.

The constraint is defined as follows: if an iterative stress state enters the region enclosed by the final complementary tensile cone, the Newton corrective step-length is scaled down so as to locate the point on the cone boundary. Figure 3.13 shows an example of this by comparing the path followed by the same stress-return with and without resorting to line search, starting from a trial state infinitesimally close to the cone boundary but external to it.

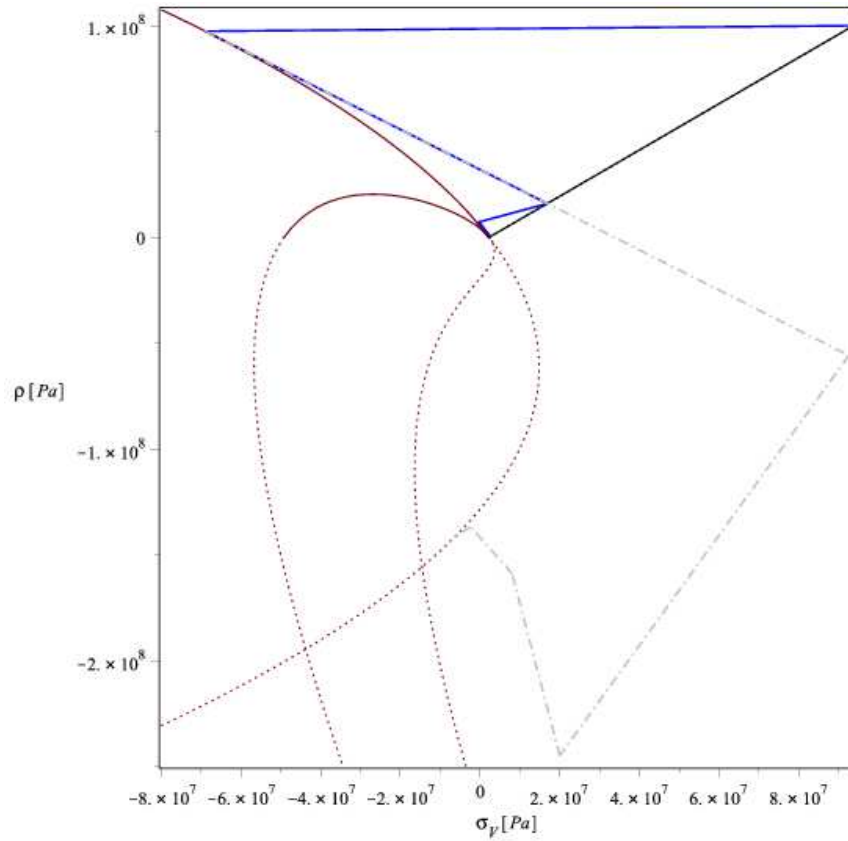


Figure 3.13: Single step stress-return along the compressive meridian plane, with (blue) and without (grey) line search. Tensile cone (black) and meridians (red) are solid in the admissible stress domain and dotted otherwise

This comparison highlights a further issue that the proposed line search strategy helps to address. When the returned stress point is located in the close vicinity of the tensile apex the potential *overshooting* from certain corrections becomes very significant, to the extent that even if the iterative procedure manages to eventually retain convergence, it does so by attaining a solution value of deviatoric radius well within the negative domain. Although this is mathematically possible, it is physically inadmissible and hence such converged solutions are to be prevented. Figure 3.14 shows in more detail the stress-return path without line search of Figure 3.13, including the evolution of the singularity contours corresponding to the intermediate iterative solutions as well as the shape of the determinant of the associated Jacobians:

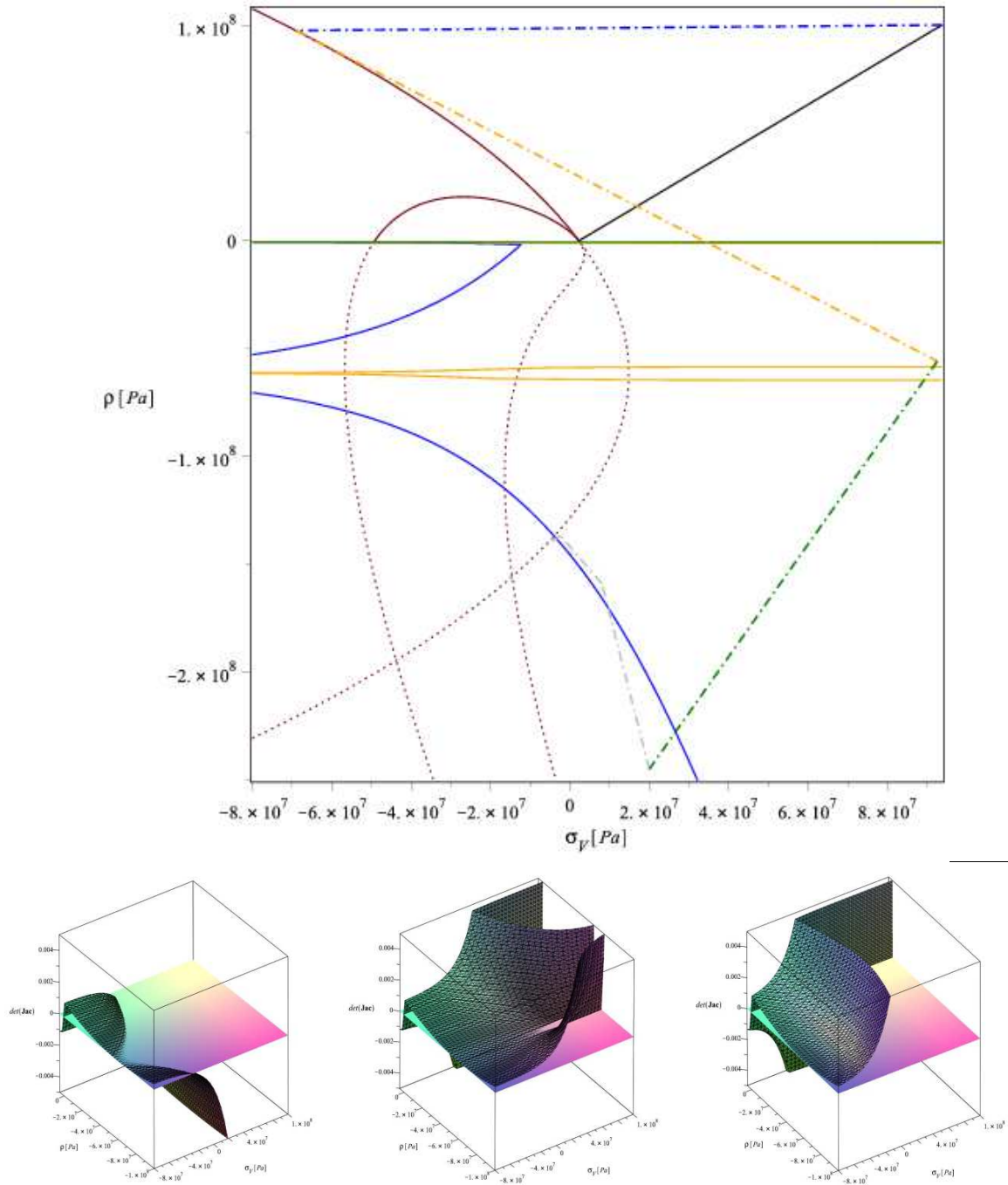


Figure 3.14: Stress-return without line search. 1<sup>st</sup> update (blue): correction (dashed), singularity contour (solid) and shape of  $\det(\mathbf{Jac})$  (bottom left). 2<sup>nd</sup> update (yellow): shape of  $\det(\mathbf{Jac})$  (bottom centre). 3<sup>rd</sup> update (green): shape of  $\det(\mathbf{Jac})$  (bottom right)

As becomes apparent from the bottom right plot of Figure 3.14, for significantly larger values of the plastic multiplier the singularity contour becomes almost coincident with the hydrostatic axis from the side of negative  $\bar{p}$ . This further reinforces the convenience of the postulated constraint, since the downscaling of an *overshot* correction ensures that it is along

a descent direction, i.e. damping prevents any iterative stress state to lie on or enter the singularity contours no matter how large the plastic multiplier.

Formally, the intersection of the final tensile cone with any meridian plane can be expressed as:

$$\bar{\sigma}_V = \frac{\bar{f}_c}{m_0} + s_t \cdot \bar{\rho} \quad (3.60)$$

with the slope elaborated as:

$$s_t = \frac{K}{2G} \frac{\sqrt{6}A_g}{m_0} \exp\left(\frac{\bar{f}_c / m_0 - \bar{f}_t / 3}{B_g \bar{f}_c}\right) \quad (3.61)$$

Hence, the downscaling can be performed explicitly if a certain check is satisfied, depending on which side of the line (3.60) the iterative stress state is located. In case the region enclosed by the cone is entered, forcing the iterative correction to lie just on the cone surface gives rise to the following expression for the damping factor:

$$\alpha^{k+1,(n+1)} = \frac{\frac{\bar{f}_c}{m_0} + s_t \cdot \bar{\rho}^{k,(n+1)} - \bar{\sigma}_V^{k,(n+1)}}{\Delta \bar{\sigma}_V^{k+1,(n+1)} - s_t \cdot \Delta \bar{\rho}^{k+1,(n+1)}} \quad (3.62)$$

which, in sight of the definition of the constraint, complies strictly with  $\alpha < 1$ .

In order to investigate if the damping factor as obtained in (3.62) can be strictly positive, Figure 3.15 shows the iterative corrective directions from points located on the final tensile cone, for the case that the starting stress points correspond to the trial state (a) or to an intermediate iterative state (b). Should the corrective direction enter the cone, then the constraint, as per its definition, would force the corrective step-length to be downscaled to zero and therefore would block the stress-return procedure. Hence, the limiting case corresponding to  $\alpha = 0$  is that where the corrective direction equals the slope (3.61):

$$\frac{\Delta \bar{\sigma}_V^{k+1,(n+1)}}{\Delta \bar{\rho}^{k+1,(n+1)}} = s_t \quad (3.63)$$

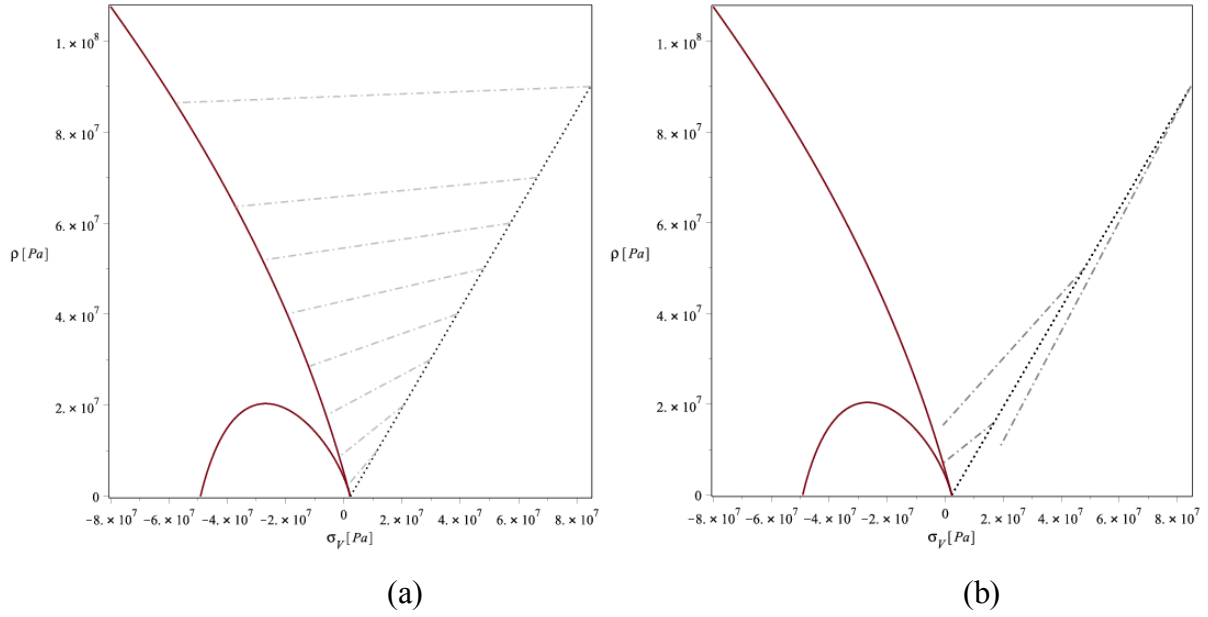


Figure 3.15: Iterative corrective directions: (a) 1<sup>st</sup> update, from trial states on the cone surface  
(b) 3<sup>rd</sup> update, from iterative states on the cone surface

For the case depicted in Figure 3.15a, (3.63) can be elaborated as:

$$s_t = \frac{K}{2G} \frac{m_V^{0,(n+1)}}{m_D^{0,(n+1)}} \quad (3.64)$$

which in turn, after combining (3.54) and (3.61), leads to the implicit relation:

$$\frac{3 \|\mathbf{J}_{2,\bar{\sigma}}\|^{tr}}{\bar{f}_c^2} + \frac{m_0}{\sqrt{6}\bar{f}_c} \left\{ \frac{\|\mathbf{J}_{2,\bar{\sigma}}\|^{tr}}{\bar{\rho}^{tr}} - \exp\left(\frac{s_t \cdot \bar{\rho}^{tr}}{B_g \bar{f}_c}\right) \right\} = 0 \quad (3.65)$$

For the compressive and tensile meridian planes, it can be shown that (3.65) can only be satisfied for  $\bar{\rho}^{tr} = 0$  and thus any trial state on the tensile cone surface will proceed on to the first correction without risk of blocking.

If the stress point under consideration is not a trial one but represents an iterative state where line search has already been activated (Figure 3.15b), with the subsequent downscaling of the corrective step-length for the point to lie on the tensile cone surface, then (3.64) must be generalised to:

$$s_t = \left( \frac{-2Gm_D \frac{\partial f_p}{\partial \bar{\rho}} r_\sigma + Km_V \frac{\partial f_p}{\partial \bar{\rho}} r_\rho - Km_V \left( 1 + 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\rho}} \right) r_f}{2Gm_D \frac{\partial f_p}{\partial \bar{\sigma}_V} r_\sigma - Km_V \frac{\partial f_p}{\partial \bar{\sigma}_V} r_\rho - 2Gm_D \left( 1 + K\Delta\lambda \frac{\partial m_V}{\partial \bar{\sigma}_V} \right) r_f} \right)^{k,(n+1)} \quad (3.66)$$

The assessment of (3.66) is cumbersome as it depends on the location of the trial stress point and the updated value of the plastic multiplier resulting from the partial stress-return up to the  $k$ -th iterative state. As shown in Figure 3.15b, it is worth noting that for trial states sufficiently ‘far away’ from the failure surface it is possible to have iterative states where, after line search activation, the subsequent corrective direction has a slope below the threshold marked by (3.66). In such cases blocking of the stress-return would ensue as a result of  $\alpha = 0$ .

A possible circumvention of this issue could be the imposition of a minimum threshold value  $\alpha_{\min}$  to allow the stress-return procedure to continue. However, since the volumetric and deviatoric trial stress coordinates necessary for the corrective slope to fall below (3.66) are generally at least 2 orders of magnitude larger than the typical average concrete tensile strength, any reasonable incremental step prescribed for analysis effectively plays the role of a cap. Hence, from a practical perspective,  $\alpha > 0$  is ensured provided that the (pseudo)time discretisation is not unreasonably coarse.

With all aforementioned considerations taken into account, the damping factor is effectively  $\alpha^{k+1,(n+1)} \in ]0,1[$  every time line search is activated in an iterative correction. Moreover, since potential iterative corrections leading to the hydrostatic axis are also prevented by the constraint definition, continuity of the Jacobian functions is also ensured within the interval defined by 2 consecutive iterative states. This continuity can be shown to satisfy Lipschitz conditions (Deuflhard, 2004) which, along with the inverse of the Jacobian being bounded, in turn imply residual contraction. Although mathematically not enough to guarantee global convergence (to do so, one would have to comply with the Wolfe conditions in terms of sufficient decrease and curvature, or prove that  $\alpha^{k+1,(n+1)}$  is within some range around a theoretical optimal value, as in Deuflhard (2004)), the residual contraction requirement is considered sufficient in the present context. Under the same step increment considerations applicable to the positive sign of the damping factor, the present choice of line search scheme

is qualitatively justified. Its inclusion in the algorithmic architecture of the standard stress-return, as well as that of the rank reduction of the residual system, is represented in Figure 3.16.

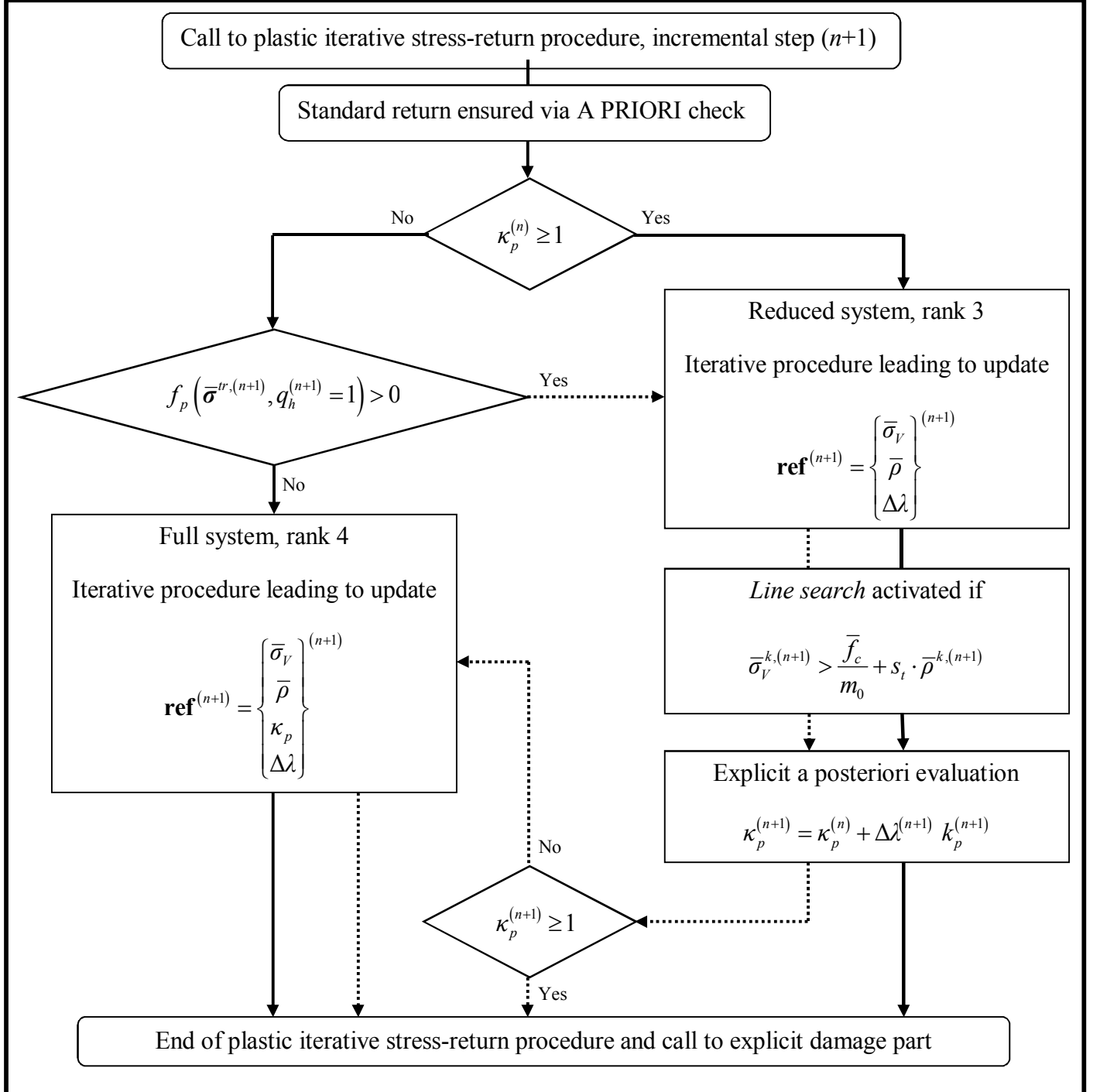


Figure 3.16: Flowchart of the standard stress-return procedure

### 3.3.2 Evaluation of algorithmic robustness

Following previous related work by Valentini and Hofstetter (2011), the algorithmic robustness of the stress-return, schematically described in Figures 3.3 and 3.16, is evaluated for a set of trial stress states distributed in a regular grid of 51 x 51 points on given meridian planes (in this case  $\bar{\theta}^{tr} = \frac{\pi}{3}$  and  $\bar{\theta}^{tr} = 0$ ). The stress-return is performed in a single step throughout. The boundaries of the grid are defined as  $\bar{\sigma}_v^{tr} \in [-80, 20]$  MPa and  $\bar{\rho}^{tr} \in [0, 40]$  MPa, with all initial values of stress, plastic strain and internal variables set to zero.

As shown in Figure 3.17, the enhanced single-step stress-return algorithm is capable of achieving convergence in 100% of the trial stress cases for both meridian planes.

Illustratively shown only for the compressive meridian plane case  $\left(\bar{\theta}^{tr} = \frac{\pi}{3}\right)$  at the bottom of

Figure 3.17, the same result is obtained if the positive boundaries of the grid are doubled in extent. This is actually sustained for up to a 7-fold extension of the grid positive boundaries, at which point certain trial stress states suffer from blockage in the stress-return due to the damping factor (3.62) dropping to zero. As commented upon in the previous section, such increments are effectively excessive for a single-step scheme of stress-return and consequently the present results are considered robust for any realistic analysis situation.

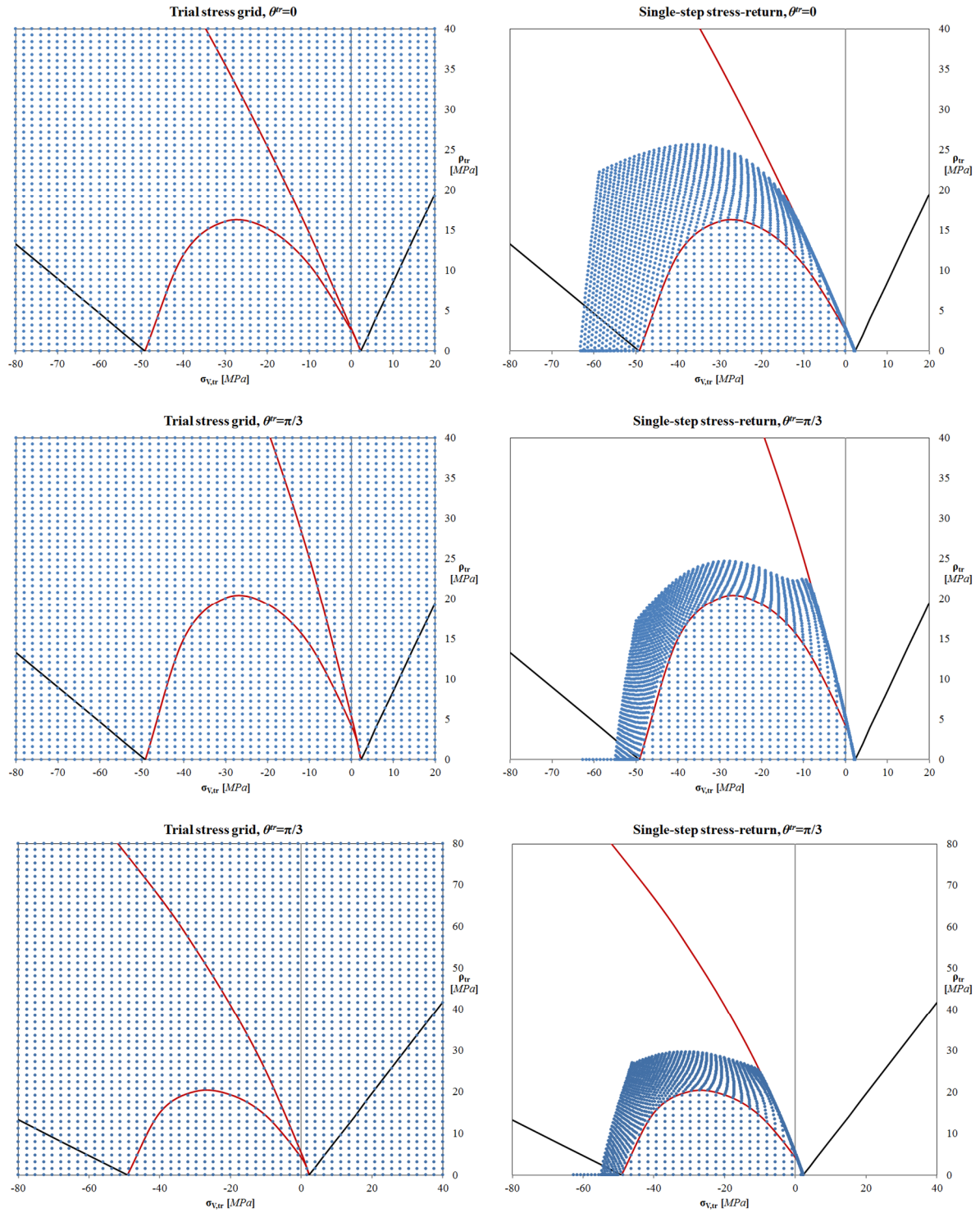


Figure 3.17: Single-step stress-returns (right) from the regular trial stress grid (left)

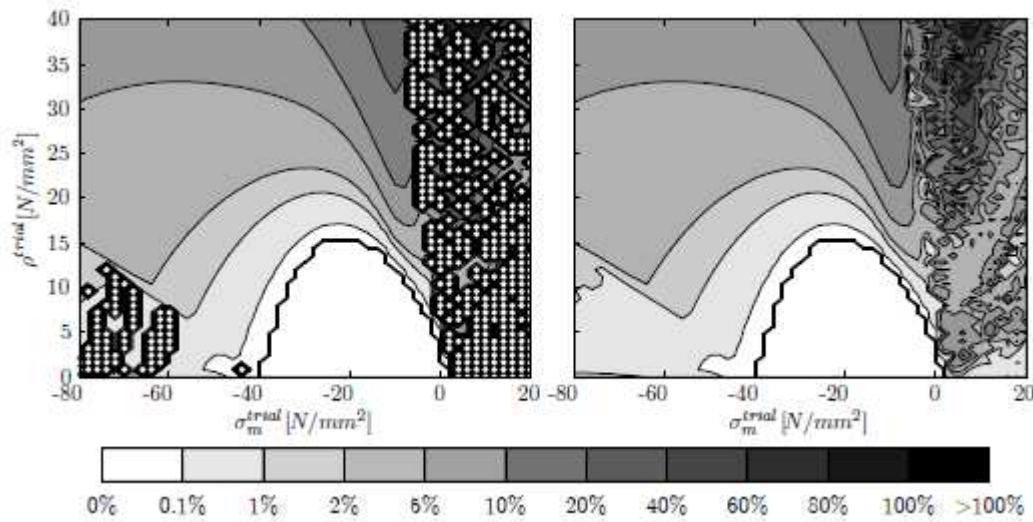


Figure 3.18: Iso-error maps for single-step stress-returns with (right) and without (left) sub-incrementation. White dots indicate points with no convergence [from Valentini and Hofstetter (2011)]

As opposed to Valentini and Hofstetter (2013), resorting to sub-incrementation was not necessary for full convergence in the currently proposed approach. In this regard, the iso-error maps of the reference for single step stress-return (Figure 3.18) show a clear correspondence between their areas of convergence failure and the complete (rank 4) formulation contours of Jacobian singularity of Figure 3.7. Incidentally, convergence fails in the areas bounded by the cones as well, as apex returns are treated differently. As comparison with Figure 3.17, if both the line search scheme and the reduced rank 3 formulation measures are deactivated for the trial grid in the compressive meridian plane with extended positive boundaries, full convergence ratio is not achieved, as shown in Figure 3.19.

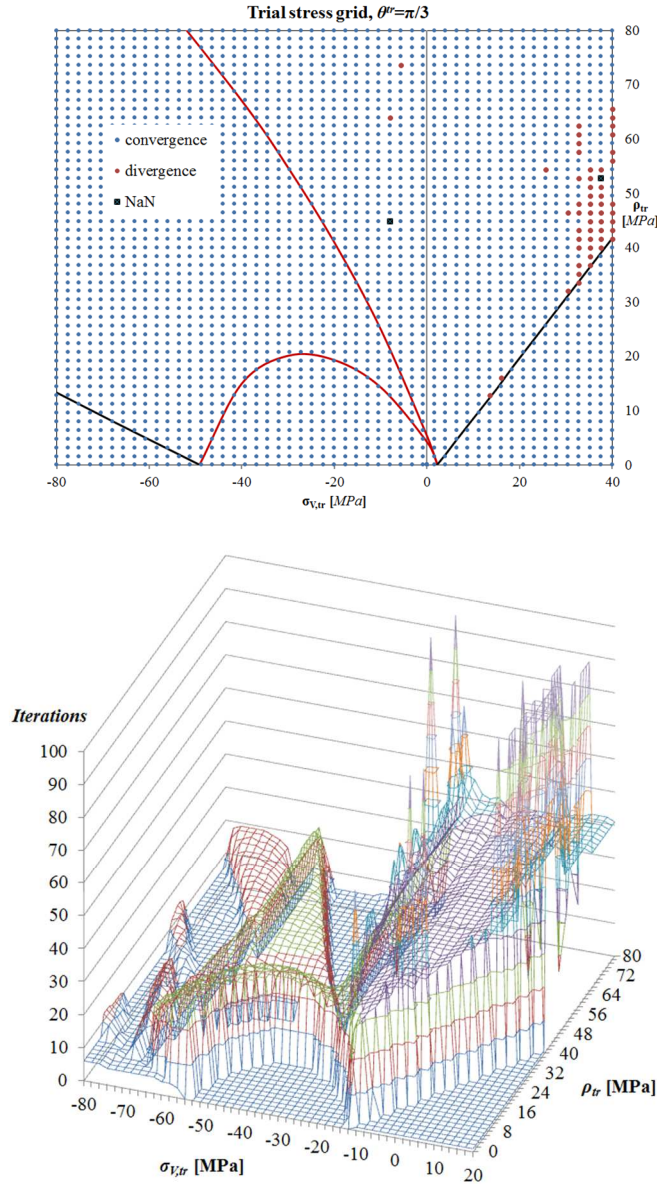


Figure 3.19: Single-step stress-returns with indication of convergence failure (top) and distribution of iterations (bottom), without line search and reduced formulation

At 54 trial stress points of the grid the iterative procedure fails to converge (either by surpassing a certain threshold of iterations or by the output becoming undefined). Moreover, the required number of iterations for converged stress-states increases significantly, as shown in Figure 3.19 for the whole grid. The proposed corrective measures drop the maximum number of iterations from 91 to 13, and the average from 20.16 to 4.53.

With the active measures, iso-error maps have also been constructed taking as reference for the exact solution the outcome of a refined sub-incrementation scheme applied to the same

trial stress grid along the compressive meridian plane. Such maps are shown in Figure 3.20 and are fully defined in the whole trial stress domain. They display the expected features: a slower increase of relative error in the hardening domain for greater distances from the elastic envelope and an acute increase of relative error in the softening domain, especially towards the sides of the *wedge* delimited by the final meridian and the tensile cone. More precisely, the former would correspond to the Jacobian singularity contour in the rank 4 formulation (as shown superimposed in Figure 3.20 top right) and the latter to the region prone to *overshooting* into the inadmissible domain of effective stresses, hence reaffirming the contribution of the proposed features to algorithmic robustness.

The algorithmic stiffness  $\Theta$ , as elaborated in Section 3.4 and ultimately obtained from the system of simultaneous equations (3.31) entering the iterative solution procedure, also entails a significant benefit in the framework of this numerical test. Resorting to sub-incrementation necessitates the updating of  $\Theta$  at every sub-incremental step, at the cost of a greater computational expense, whereas here it only requires updating at the end of the single incremental step.

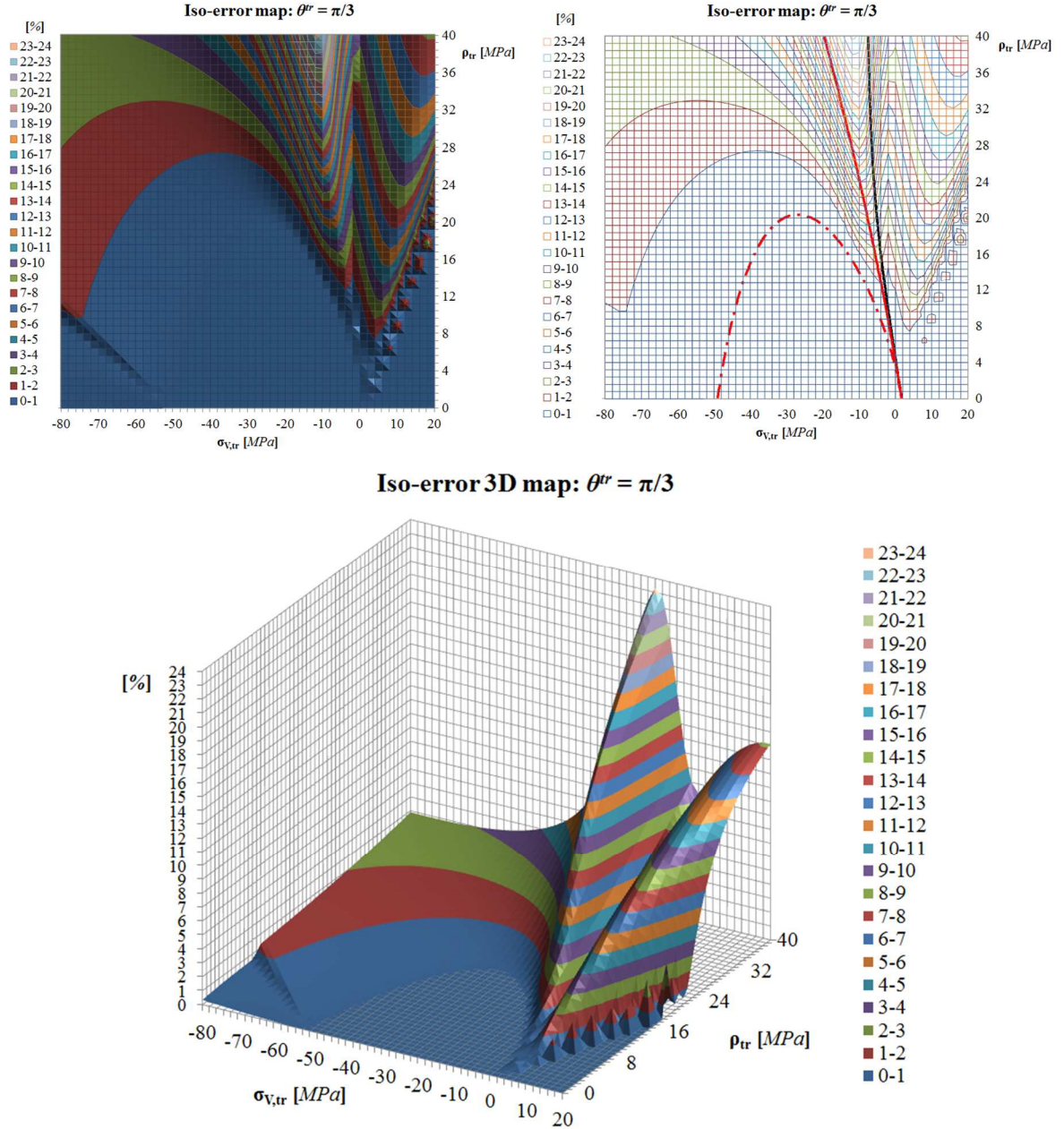


Figure 3.20: 2D (top) and 3D (bottom) iso-error maps for single step stress-return on the compressive meridian plane. At the top right, meridians (red) and the singularity contour of  $\mathbf{Jac}_0$  (black) are superimposed for comparison

### 3.3.3 Proposal for modification of plastic flow

Since the Haigh-Westergaard coordinates given by (3.1) to (3.3) correspond to a cylindrical coordinate system, the hydrostatic axis is by definition not part of the system regularity region, i.e. along the hydrostatic axis Lode's angle remains undefined. Following Grassl *et al.* (2013),  $\bar{\theta}^{tr} = 0$  has been arbitrarily enforced for any trial state with  $\bar{\rho}^{tr} = 0$  in

the previous elaborations. Therefore, for pure hydrostatic stress states, the evolution of the internal strain-like hardening variable according to (3.17) always takes place as if the stress-return were evolving along the tensile meridian plane, regardless of the orientation that would follow from (3.3) should there be a small perturbation in the deviatoric component.

This becomes apparent when inspecting the compressive apex returns shown in Figure 3.13 for the compressive and tensile meridian planes (the volumetric shift of the tensile apex is negligible, making the differences between meridian planes unappreciable on that end). In the absence of any further difference, setting  $\bar{\theta} = 0$  in (3.17) instead of  $\bar{\theta} = \pi/3$  gives rise to a quadruple increase in the evolution rate of  $\kappa_p$ . Consequently, the returned states from purely hydrostatic trial states belonging to the stress grid of the compressive meridian plane display a discontinuity in the segment of the hydrostatic axis in the vicinity of the compressive apex.

In order to address this, and to accommodate the intuitive requirement that the returned stress grid should tend to the same volumetric values when approaching the hydrostatic axis from any meridian plane, the following modification is proposed in the rate equation (3.17):

$$\dot{\kappa}_p(\bar{\sigma}, \kappa_p) = \dot{\lambda} k_p(\bar{\sigma}, \kappa_p) = \frac{\dot{\lambda} \|\mathbf{m}\|}{x_h} (r_2)^2 \quad (3.67)$$

with:

$$r_2 = \frac{4(1 - e_\theta^2) \cos^2 \bar{\theta} + (2e_\theta - 1)^2}{2(1 - e_\theta^2) \cos \bar{\theta} + (2e_\theta - 1) \sqrt{4(1 - e_\theta^2) \cos^2 \bar{\theta} + 5e_\theta^2 - 4e_\theta}} \quad (3.68)$$

playing formally a similar role to the Willam & Warnke function (3.6), shaping in this case the evolution of  $\kappa_p$  in the deviatoric plane by means of the eccentricity  $e_\theta$ . If  $e_\theta$  is defined in such a way that it tends to unity as the deviatoric radius tends to zero, and it attains the value 1/2 beyond a certain threshold around the hydrostatic axis, then, substituting in (3.68):

$$\begin{cases} r_2 = 1 & \text{if } e_\theta = 1 \\ r_2 = 2 \cos(\bar{\theta}) & \text{if } e_\theta = \frac{1}{2} \end{cases} \quad (3.69)$$

For pure hydrostatic cases, the returned volumetric stress component would tend to the value obtained with  $\bar{\theta} = \frac{\pi}{3}$  from every possible meridian plane. The original formulation (3.17) is retrieved once the threshold has been crossed and, for intermediate cases, the influence of

Lode's angle on  $\kappa_p$  is modulated from a circular to a quadratic triangular cross-section in the deviatoric plane, as prescribed by (3.68).

The aforementioned threshold is defined, on a generic meridian plane, by means of a polar system  $(\zeta, \psi)$  around the initial compressive apex  $\bar{\sigma}_{V,apex,C}^{(0)}$ , obtained as the negative real root of equation (3.35) for  $q_h = q_{h0}$ . Such a system is schematically represented in Figure 3.21a and relates to the in-plane Haigh-Westergaard coordinates as follows:

$$\zeta = \sqrt{\bar{\rho}^2 + 3\left(\bar{\sigma}_V - \bar{\sigma}_{V,apex,C}^{(0)}\right)^2} \quad (3.70)$$

$$\tan \psi = \begin{cases} -\frac{\bar{\rho}}{\left(\bar{\sigma}_V - \bar{\sigma}_{V,apex,C}^{(0)}\right)}, & \text{if } \zeta \neq 0 \wedge \bar{\sigma}_V \leq \bar{\sigma}_{V,apex,C}^{(0)} \\ \frac{\bar{\rho}}{\left(\bar{\sigma}_V - \bar{\sigma}_{V,apex,C}^{(0)}\right)}, & \text{if } \zeta \neq 0 \wedge \bar{\sigma}_V > \bar{\sigma}_{V,apex,C}^{(0)} \end{cases} \quad (3.71)$$

Hence, by taking the initial compressive cone as the threshold, it follows that:

$$\tan \psi_c = -\frac{1}{s_c^{(0)}} \quad (3.72)$$

with  $s_c^{(0)}$  representing the slope of the cone. Similar elaborations to (3.61) lead in this case to:

$$s_c^{(0)} = \frac{K}{2G} \cdot \frac{\frac{4}{\bar{f}_c}(1-q_{h0})^2 \left(\frac{\bar{\sigma}_{V,apex,C}^{(0)}}{\bar{f}_c}\right)^3 + \frac{q_{h0}^2}{\bar{f}_c} A_g \exp\left(\frac{\bar{\sigma}_{V,apex,C}^{(0)} - \frac{\bar{f}_t}{3}}{B_g \bar{f}_c}\right)}{(1-q_{h0})^2 \frac{4}{\sqrt{6}\bar{f}_c} \left(\frac{\bar{\sigma}_{V,apex,C}^{(0)}}{\bar{f}_c}\right)^3 + \frac{\sqrt{6}}{\bar{f}_c}(1-q_{h0}) \left(\frac{\bar{\sigma}_{V,apex,C}^{(0)}}{\bar{f}_c}\right)^2 + q_{h0}^2 \frac{m_0}{\sqrt{6}\bar{f}_c}} \quad (3.73)$$

This allows for the introduction of the transition function:

$$R = \begin{cases} \frac{\tan \psi}{\tan \psi_c}, & \text{if } \psi < \psi_c \\ 1, & \text{if } \psi \geq \psi_c \end{cases} \quad (3.74)$$

and, finally, the formal definition of the eccentricity:

$$e_\theta = 1 - \frac{R}{2}(R^2 - 3R + 3) \quad (3.75)$$

based on a similar evolution law as (3.16) and depicted in Figure 3.21b.

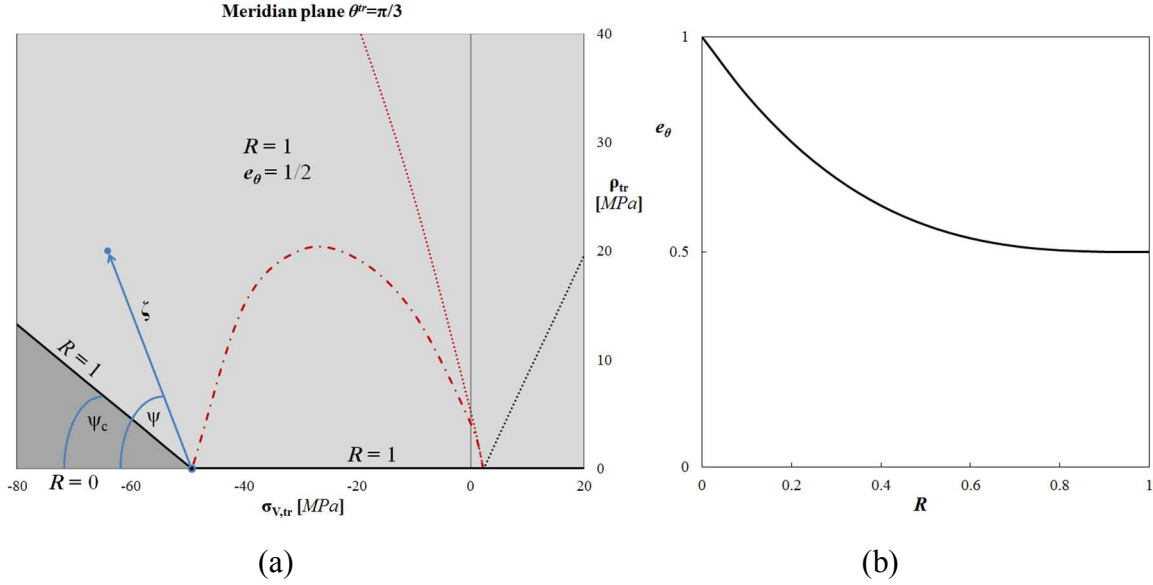


Figure 3.21: (a) Local polar system on the compressive meridian plane; the dark shaded area corresponds to the domain affected by the evolution of  $R$  (b) Evolution of the eccentricity with  $R$

Similar to the hydrostatic axis in Haigh-Westergaard coordinates, the rotation axis of the polar system is not part of its regularity region and hence the initial compressive apex (i.e.  $\zeta = 0$ ) requires enforcing  $\psi = \psi_c$ . By doing so,  $R$  remains continuous and bounded in the range  $[0, 1]$ , the boundary  $R=1$  being the piecewise linear solid line in Figure 3.21a, where in the light shaded area (including the boundary) the original formulation is retrieved. Consequently, as per (3.75),  $e_\theta$  remains bounded between 1 (on the hydrostatic axis) and  $\frac{1}{2}$  (on the surface of the initial compressive cone). The fact that the  $R=1$  boundary includes the initial compressive apex entails no conflict, as this relates to a neutral loading situation, and hence  $\Delta\lambda = 0$  with  $f_p = 0$  regardless of the definition of  $k_p$ . Also, the  $C^1$  discontinuity of  $R$  along the initial compressive cone poses no additional difficulty when computing the appropriate elements of the Jacobian matrix affected by the inclusion of  $r_2$ , as this jump at  $\psi = \psi_c$  is bounded and eventually cancelled by  $\frac{\partial e_\theta}{\partial R} \Big|_{\psi=\psi_c} = 0$ . The Jacobian for the standard

and iterative apex returns must be modified in line with the new dependencies introduced by substituting (3.68)-(3.75) in (3.67). Figure 3.22 shows the same trial stress grid used in the previous section (whereby the trial point density has been doubled) for single-step stress-

returns along  $\bar{\theta}^{tr} = 0$  and  $\bar{\theta}^{tr} = \pi/3$ .

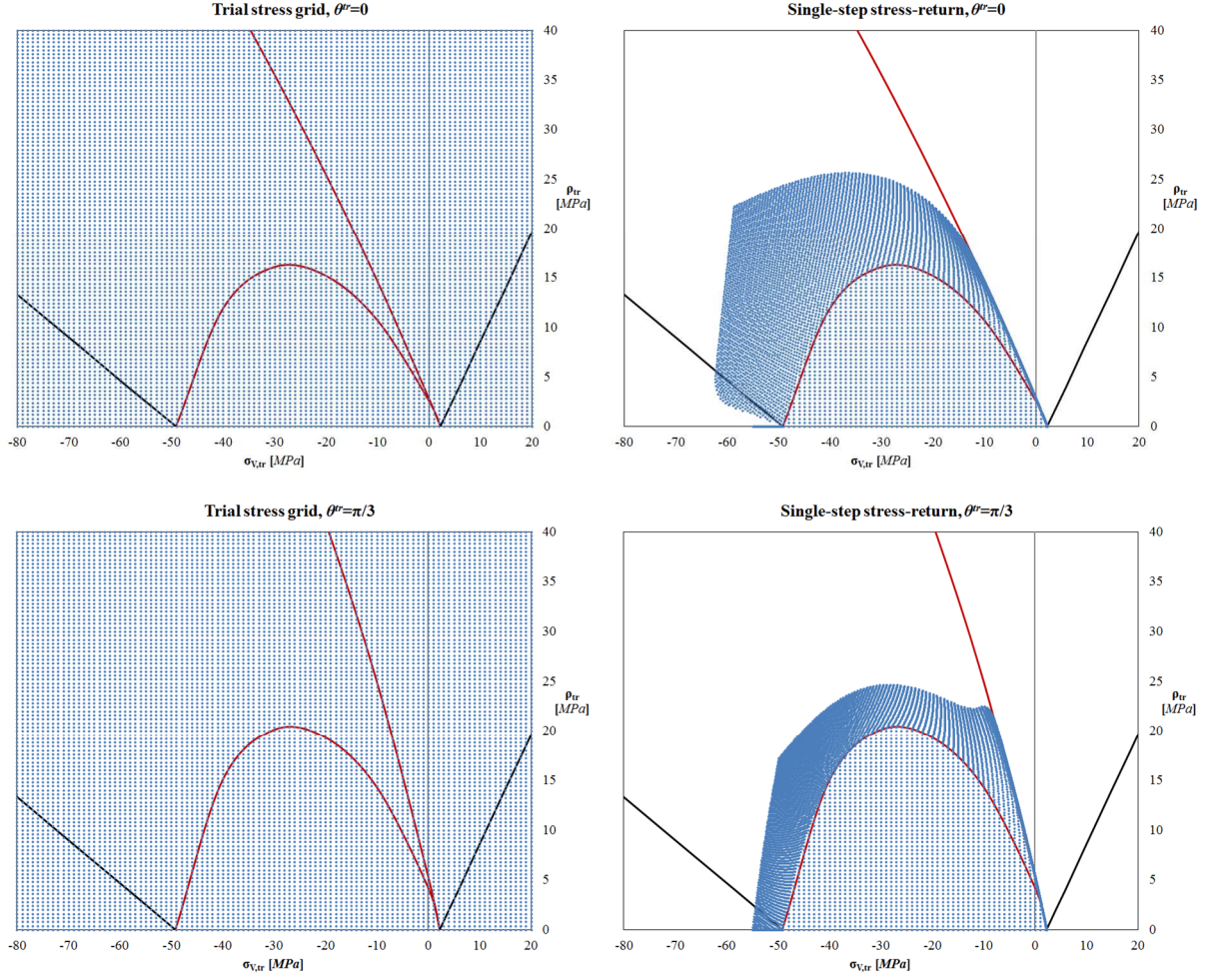


Figure 3.22: Single-step stress-returns (right) from the regular trial stress grid (left) along the tensile (top) and compressive (bottom) meridian plane, including elastic envelope and final meridian (red) as well as initial tensile and compressive cones (black)

As expected, convergence as such is not affected by the inclusion of  $r_2$  and, inside the initial compressive cone of the compressive meridian plane, the plastic hardening evolution is slowed down, tending towards the same hydrostatic returned stress states as in the tensile meridian plane. There is, however, an apparent gap between stress points returned to the compressive apex and stress points returned to its vicinity but on the yield surface. This is due to the progressive slowdown of the yield surface evolution with the proximity of the trial stress points to the hydrostatic axis. In fact, the closer a trial stress point is to this axis, the less does the compressive cone shift in stress space, in the rate given by function  $R$  (3.74), which further increases the number of cases where the *a posteriori* check (3.40) is satisfied. This in turn means that more stress points end up returning to the compressive apex as compared to the standard formulation without  $r_2$ . Illustratively, this is shown in Figure 3.23,

where the stress-return of trial points with the same volumetric component ( $\bar{\sigma}_V = -80\text{MPa}$  and  $\bar{\sigma}_V = -70\text{MPa}$ ) but varying deviatoric radius is tracked.

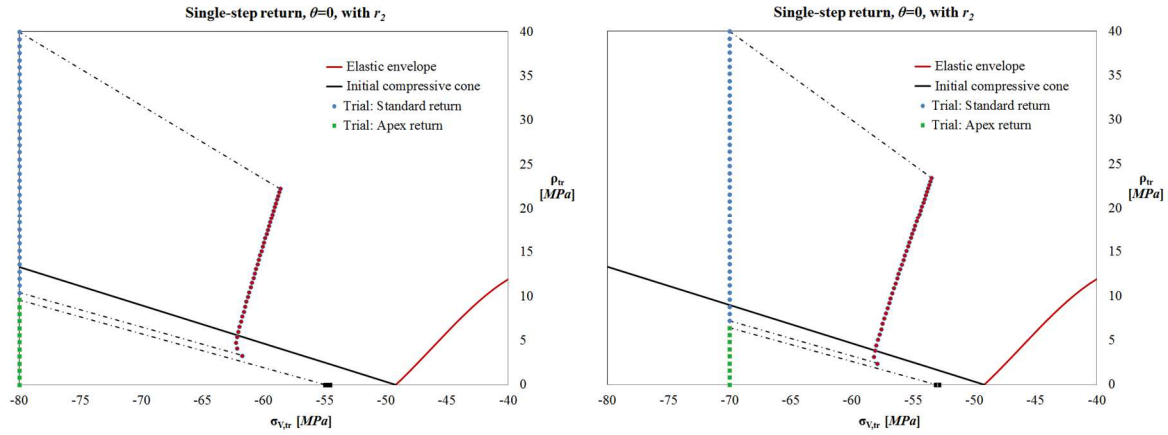


Figure 3.23: Single-step stress-returns of trial stress points in the same deviatoric section

Although the convergence ratio is not affected, the convergence rate does decay, as the number of iterations increases notably, particularly for stress points that only return to the apex because of the hardening slowdown. With this in consideration, and although it is desirable to reconcile the hydrostatic response in different meridian planes, the current proposal is not included in the final implemented version of the model for application purposes.

### 3.4 Algorithmic elasto-plastic-damage stiffness

As is well established in the literature (Nagtegaal, 1982; Simo and Taylor, 1985), achieving a quadratic convergence rate in a full Newton scheme of the global equilibrium iterative procedure necessitates from resorting to the algorithmic stiffness  $\Theta$  instead of the material tangential stiffness  $\mathbf{D}$ . The global stiffness matrix is then defined, for incremental step  $(n+1)$  and iteration  $(i)$ , as:

$$\mathbf{K}^{i,(n+1)} = \int_V \mathbf{B}^T \Theta^{(n+1)} (\boldsymbol{\varepsilon}^{i,(n+1)}) \mathbf{B} dV \quad (3.76)$$

where the more usual vectorial notation is used in (3.76), and only the geometrically linear term is shown for simplicity, with the standard B-matrix containing the derivatives of shape functions. While  $\mathbf{D}$  expresses the infinitesimal change in stresses due to a perturbation in the current strains,  $\Theta$  represents the infinitesimal change in the output of the stress evaluation algorithm due to a perturbation in the current finite strain increment. That is,  $\mathbf{D}$  is obtained by differentiation of the constitutive law whereas  $\Theta$  is obtained by differentiation of the

numerical algorithm used for the update of stresses (Jirásek, 2014). This is schematically shown in Figure 3.24, from where it can be deduced that:

$$\Theta^{(n+1)} \equiv \left( \frac{\partial \sigma}{\partial \varepsilon} \right)^{(n+1)} \quad (3.77)$$

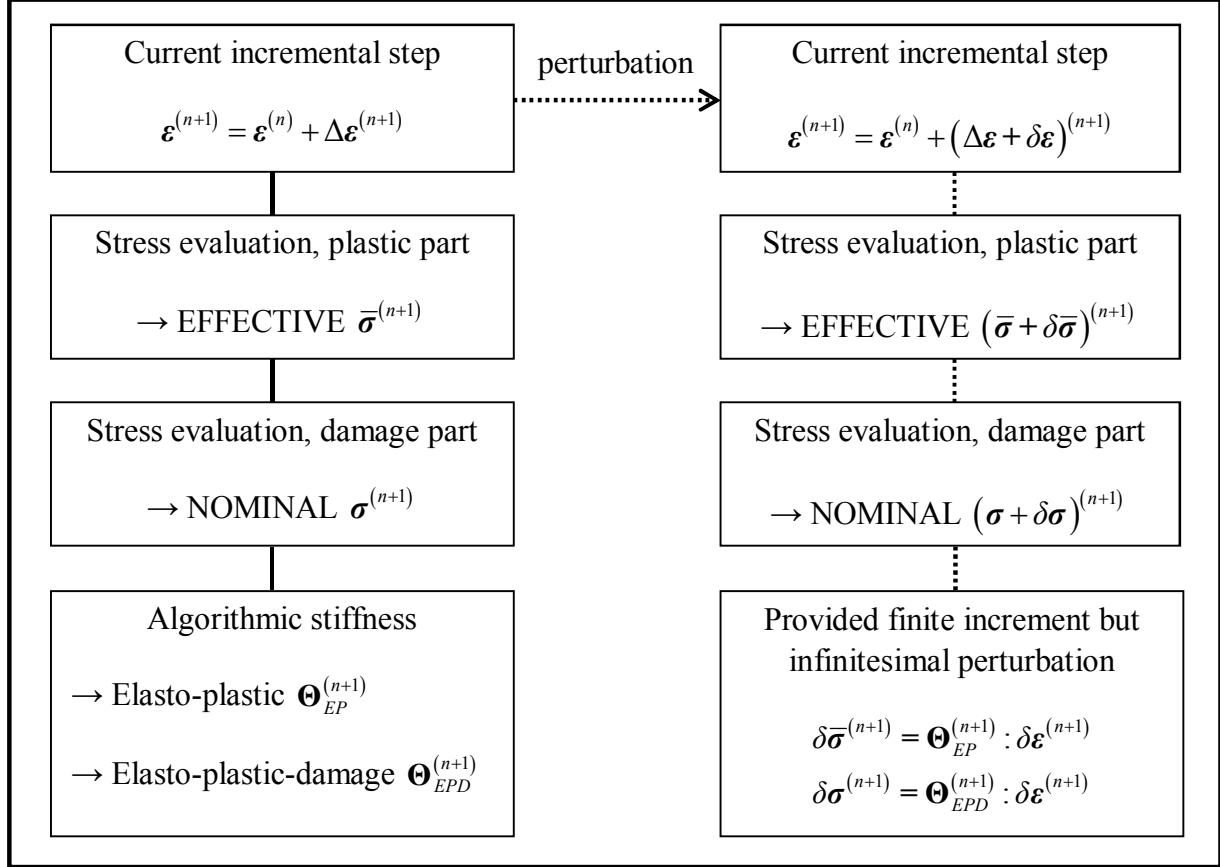


Figure 3.24: Meaning of  $\Theta$  as the relation of  $\delta\sigma / \delta\bar{\sigma}$  to  $\delta\varepsilon$

In the present context, the stress evaluation corresponds to the output of CDPM, as described in section 3.2. Following Grassl and Jirásek (2006a), the consistent differentiation of this evaluation algorithm can be subdivided into the plastic part, leading to  $\Theta_{EP}$ , and the damage part, leading to  $\Theta_{EPD}$ , where the incremental step index  $(n+1)$  is dropped for clarity in this section.

Since the framework for the plastic iterative stress-return is the space of principal effective stresses in the Haigh-Westergaard coordinate system, the resulting perturbations in the effective stress Cartesian components are ultimately expressed in terms of perturbations in principal values as well as principal directions (by differentiation of  $\bar{\sigma}$  as expressed in Figure 3.2). The former are in turn a function of perturbations in the returned state Haigh-

Westergaard coordinates and so, as elaborated in Jirásek and Zimmermann (1998a), the following relations ensue:

$$\begin{aligned}\delta\bar{\sigma}_{11} &= \delta\bar{\sigma}_1 = \delta\bar{\sigma}_V + \sqrt{\frac{2}{3}} \cos \bar{\theta}^{tr} \delta\bar{\rho} - \sqrt{\frac{2}{3}} \bar{\rho} \sin \bar{\theta}^{tr} \delta\bar{\theta}^{tr} \\ \delta\bar{\sigma}_{22} &= \delta\bar{\sigma}_2 = \delta\bar{\sigma}_V + \sqrt{\frac{2}{3}} \cos \left( \bar{\theta}^{tr} - \frac{2\pi}{3} \right) \delta\bar{\rho} - \sqrt{\frac{2}{3}} \bar{\rho} \sin \left( \bar{\theta}^{tr} - \frac{2\pi}{3} \right) \delta\bar{\theta}^{tr} \\ \delta\bar{\sigma}_{33} &= \delta\bar{\sigma}_3 = \delta\bar{\sigma}_V + \sqrt{\frac{2}{3}} \cos \left( \bar{\theta}^{tr} + \frac{2\pi}{3} \right) \delta\bar{\rho} - \sqrt{\frac{2}{3}} \bar{\rho} \sin \left( \bar{\theta}^{tr} + \frac{2\pi}{3} \right) \delta\bar{\theta}^{tr}\end{aligned}\quad (3.78)$$

$$\begin{aligned}\delta\bar{\sigma}_{12} &= \left( \frac{\bar{\sigma}_1 - \bar{\sigma}_2}{2(\varepsilon_{e1}^{tr} - \varepsilon_{e2}^{tr})} \right) \cdot \delta\gamma_{12} \\ \delta\bar{\sigma}_{13} &= \left( \frac{\bar{\sigma}_1 - \bar{\sigma}_3}{2(\varepsilon_{e1}^{tr} - \varepsilon_{e3}^{tr})} \right) \cdot \delta\gamma_{13} \\ \delta\bar{\sigma}_{23} &= \left( \frac{\bar{\sigma}_2 - \bar{\sigma}_3}{2(\varepsilon_{e2}^{tr} - \varepsilon_{e3}^{tr})} \right) \cdot \delta\gamma_{23}\end{aligned}\quad (3.79)$$

where  $\varepsilon_{eI}^{tr}$  are the principal trial elastic strains and  $\delta\gamma_{IJ}$  are the (engineering) shear components of  $\delta\boldsymbol{\varepsilon}$  in  $\mathbf{n}_I$  base (Figure 3.2), i.e. the Eigenbase of the trial/returned state without perturbation.

The infinitesimal changes in shear stress components (3.79) follow very specific proportionality relations with  $\delta\gamma_{IJ}$ , namely the ones that ensure coaxiality between rotating stresses and strains (as in Jirásek and Bazant (2002)). As shown in Grassl and Jirásek (2006a), and in part due to such coaxiality entailing that  $\bar{\theta}^{tr}$  be the same in stress and strain space, the case of two coinciding  $\varepsilon_{eI}^{tr}$  can be accommodated by doing:

$$\begin{aligned}\delta\bar{\sigma}_{12} &= \frac{\bar{\rho}}{2\rho_e^{tr}} \cdot \delta\gamma_{12} \quad \text{if } \varepsilon_{e1}^{tr} = \varepsilon_{e2}^{tr} \\ &\text{or} \\ \delta\bar{\sigma}_{23} &= \frac{\bar{\rho}}{2\rho_e^{tr}} \cdot \delta\gamma_{23} \quad \text{if } \varepsilon_{e2}^{tr} = \varepsilon_{e3}^{tr}\end{aligned}\quad (3.80)$$

where  $\rho_e^{tr}$  is defined as the norm of the deviatoric part of the trial elastic strains:

$$\rho_e^{tr} = \|\mathbf{e}_e^{tr}\| \quad (3.81)$$

The case of three identical  $\varepsilon_{eI}^{tr}$  corresponds to an apex return along the hydrostatic axis and is discussed at the end of this section.

The infinitesimal changes in normal stress components (3.78) need  $\delta\bar{\sigma}_V$ ,  $\delta\bar{\rho}$  and  $\delta\bar{\theta}^{tr}$  to be expressed as a function of the strain perturbations. By recalling that, through (3.79),  $\bar{\theta}^{tr}$  is defined identically in the strain space from (3.3) and that  $\bar{\sigma}_V$  and  $\bar{\rho}$  are obtained by solving the 4 simultaneous equations (3.31), consistent differentiation leads to:

$$\delta\bar{\theta}^{tr} = \frac{\sqrt{3}}{2J_{e2}^{2.5} \sin(3\bar{\theta}^{tr})} \left( \frac{3}{2} J_{e3} \mathbf{e}_e^{tr} - J_{e2} \mathbf{e}_e^{tr} \cdot \mathbf{e}_e^{tr} \right) : \delta \mathbf{e} \quad (3.82)$$

$$\begin{Bmatrix} \delta\bar{\sigma}_V \\ \delta\bar{\rho} \\ \delta\kappa_p \\ \delta\lambda \end{Bmatrix} = \begin{bmatrix} 1 + K\Delta\lambda \frac{\partial m_V}{\partial \bar{\sigma}_V} & K\Delta\lambda \frac{\partial m_V}{\partial \bar{\rho}} & K\Delta\lambda \frac{\partial m_V}{\partial \kappa_p} & Km_V \\ 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\sigma}_V} & 1 + 2G\Delta\lambda \frac{\partial m_D}{\partial \bar{\rho}} & 2G\Delta\lambda \frac{\partial m_D}{\partial \kappa_p} & 2Gm_D \\ -\Delta\lambda \frac{\partial k_p}{\partial \bar{\sigma}_V} & -\Delta\lambda \frac{\partial k_p}{\partial \bar{\rho}} & 1 - \Delta\lambda \frac{\partial k_p}{\partial \kappa_p} & -k_p \\ \frac{\partial f_p}{\partial \bar{\sigma}_V} & \frac{\partial f_p}{\partial \bar{\rho}} & \frac{\partial f_p}{\partial \kappa_p} & 0 \end{bmatrix}^{-1} \cdot \begin{Bmatrix} K\delta : \delta \mathbf{e} \\ \frac{2G}{\bar{\rho}^{tr}} \mathbf{s}^{tr} : \delta \mathbf{e} \\ 0 \\ -\frac{\partial f_p}{\partial \bar{\theta}} \delta\bar{\theta}^{tr} \end{Bmatrix} \quad (3.83)$$

with  $J_{e2}$  and  $J_{e3}$  being deviatoric strain invariants, and  $\delta \mathbf{e}$  being the deviatoric part of the strain perturbation. Substitution of (3.82) and (3.83) back into (3.78) together with (3.79) allows for the linear expression:

$$\delta\bar{\sigma}_{IJ} = (\mathbf{\Theta}_{EP})_{IJ} : \delta \varepsilon_{IJ} \quad (3.84)$$

in  $\mathbf{n}_I$  base for the current incremental step. Recalling from Figure 3.2 that the spectral matrix can be stored and retrieved from the trial elastic state to perform a change of base, one can finally express the relation between infinitesimal changes in Cartesian base:

$$\delta\bar{\sigma} = \mathbf{\Theta}_{EP} : \delta \mathbf{e} \quad (3.85)$$

The details about the structure of the spectral matrix and the necessary modifications to work with Voigt notation instead of full tensor notation can be found in Jirásek and Zimmermann (1998a) or Huber (2006).

While the described procedure is systematic and valid for the regular range  $0 < \bar{\theta} < \frac{\pi}{3}$  in the principal space where Eigenvalues are ordered  $I \geq II \geq III$ , the provisions given by (3.80)-

(3.81) are insufficient when the stress-return takes place along the compressive ( $\bar{\theta}^{tr} = \frac{\pi}{3}$ ) or the tensile ( $\bar{\theta}^{tr} = 0$ ) meridian planes. In such cases with two coinciding principal values,  $\delta\bar{\theta}^{tr}$  as given by (3.82) remains undefined and further provisions are needed to compute (3.78). Based on similar arguments as those behind (3.80)-(3.81), the following remedy is proposed hereafter.

The differences between consistently differentiated principal effective stresses can be obtained directly from (3.78) and read generally:

$$\begin{aligned}\delta\bar{\sigma}_1 - \delta\bar{\sigma}_2 &= \sqrt{\frac{2}{3}} \delta\bar{\rho} \left[ \cos\bar{\theta}^{tr} - \cos\left(\bar{\theta}^{tr} - \frac{2\pi}{3}\right) \right] - \sqrt{\frac{2}{3}} \bar{\rho} \delta\bar{\theta}^{tr} \left[ \sin\bar{\theta}^{tr} - \sin\left(\bar{\theta}^{tr} - \frac{2\pi}{3}\right) \right] \\ \delta\bar{\sigma}_2 - \delta\bar{\sigma}_3 &= \sqrt{\frac{2}{3}} \delta\bar{\rho} \left[ \cos\left(\bar{\theta}^{tr} - \frac{2\pi}{3}\right) - \cos\left(\bar{\theta}^{tr} + \frac{2\pi}{3}\right) \right] - \sqrt{\frac{2}{3}} \bar{\rho} \delta\bar{\theta}^{tr} \left[ \sin\left(\bar{\theta}^{tr} - \frac{2\pi}{3}\right) - \sin\left(\bar{\theta}^{tr} + \frac{2\pi}{3}\right) \right]\end{aligned}\quad (3.86)$$

Substituting  $\bar{\theta}^{tr} = \frac{\pi}{3}$  in  $\delta\bar{\sigma}_1 - \delta\bar{\sigma}_2$  and  $\bar{\theta}^{tr} = 0$  in  $\delta\bar{\sigma}_2 - \delta\bar{\sigma}_3$ , and considering that  $\delta\bar{\sigma}_I - \delta\bar{\sigma}_J = \delta(\bar{\sigma}_I - \bar{\sigma}_J)$  holds in the present framework of linearisations around the current returned state, gives rise to:

$$\begin{aligned}\delta\bar{\theta}^{tr} &= \frac{\delta(\bar{\sigma}_2 - \bar{\sigma}_3)}{\sqrt{2}\bar{\rho}} = \frac{\delta\bar{\sigma}_2 - \delta\bar{\sigma}_3}{\sqrt{2}\bar{\rho}} \quad \text{if } \bar{\theta}^{tr} = 0 \\ \delta\bar{\theta}^{tr} &= -\frac{\delta(\bar{\sigma}_1 - \bar{\sigma}_2)}{\sqrt{2}\bar{\rho}} = -\frac{\delta\bar{\sigma}_1 - \delta\bar{\sigma}_2}{\sqrt{2}\bar{\rho}} \quad \text{if } \bar{\theta}^{tr} = \frac{\pi}{3}\end{aligned}\quad (3.87)$$

By combining (3.79) and (3.80):

$$\begin{aligned}\frac{\bar{\sigma}_2 - \bar{\sigma}_3}{(\varepsilon_{e2}^{tr} - \varepsilon_{e3}^{tr})} &= \frac{\bar{\rho}}{\rho_e^{tr}} \quad \text{if } \bar{\theta}^{tr} = 0 \\ \frac{\bar{\sigma}_1 - \bar{\sigma}_2}{(\varepsilon_{e1}^{tr} - \varepsilon_{e2}^{tr})} &= \frac{\bar{\rho}}{\rho_e^{tr}} \quad \text{if } \bar{\theta}^{tr} = \frac{\pi}{3}\end{aligned}\quad (3.88)$$

differentiating consistently (3.88) leads to:

$$\begin{aligned}\delta(\bar{\sigma}_2 - \bar{\sigma}_3) &= \frac{\bar{\rho}}{\rho_e^{tr}} \delta(\varepsilon_{e2}^{tr} - \varepsilon_{e3}^{tr}) = \frac{\bar{\rho}}{\rho_e^{tr}} (\delta\varepsilon_{e2}^{tr} - \delta\varepsilon_{e3}^{tr}) \quad \text{if } \bar{\theta}^{tr} = 0 \\ \delta(\bar{\sigma}_1 - \bar{\sigma}_2) &= \frac{\bar{\rho}}{\rho_e^{tr}} \delta(\varepsilon_{e1}^{tr} - \varepsilon_{e2}^{tr}) = \frac{\bar{\rho}}{\rho_e^{tr}} (\delta\varepsilon_{e1}^{tr} - \delta\varepsilon_{e2}^{tr}) \quad \text{if } \bar{\theta}^{tr} = \frac{\pi}{3}\end{aligned}\quad (3.89)$$

Since  $\boldsymbol{\varepsilon}_e^{tr} = \boldsymbol{\varepsilon}^{(n)} + \Delta\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p^{(n)}$  it follows that  $\delta\boldsymbol{\varepsilon}_e^{tr} = \delta\boldsymbol{\varepsilon}$ , and therefore, in  $\mathbf{n}_I$  base, (3.89) can be reformulated as:

$$\begin{aligned} (\delta\bar{\sigma}_2 - \delta\bar{\sigma}_3) &= \frac{\bar{\rho}}{\rho_e^{tr}} \boldsymbol{\delta}_{23} : \delta\boldsymbol{\varepsilon} & \text{if } \bar{\theta}^{tr} = 0 \\ (\delta\bar{\sigma}_1 - \delta\bar{\sigma}_2) &= \frac{\bar{\rho}}{\rho_e^{tr}} \boldsymbol{\delta}_{12} : \delta\boldsymbol{\varepsilon} & \text{if } \bar{\theta}^{tr} = \frac{\pi}{3} \end{aligned} \quad (3.90)$$

with the matrix representation of  $\boldsymbol{\delta}_{12}$  and  $\boldsymbol{\delta}_{23}$  being:

$$\begin{aligned} \boldsymbol{\delta}_{23} &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \\ \boldsymbol{\delta}_{12} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{aligned} \quad (3.91)$$

Finally, substitution of (3.91) back into (3.87) provides the sought relation:

$$\begin{aligned} \delta\bar{\theta}^{tr} &= \frac{1}{\sqrt{2}\rho_e^{tr}} \boldsymbol{\delta}_{23} : \delta\boldsymbol{\varepsilon} & \text{if } \bar{\theta}^{tr} = 0 \\ \delta\bar{\theta}^{tr} &= -\frac{1}{\sqrt{2}\rho_e^{tr}} \boldsymbol{\delta}_{12} : \delta\boldsymbol{\varepsilon} & \text{if } \bar{\theta}^{tr} = \frac{\pi}{3} \end{aligned} \quad (3.92)$$

The results (3.92) complement (3.82) for the cases  $\bar{\theta}^{tr} = 0$  and  $\bar{\theta}^{tr} = \frac{\pi}{3}$ , allowing to follow the aforementioned steps to obtain (3.84) in  $\mathbf{n}_I$  base and then (3.85) upon change of base on any meridian plane.

To incorporate the effect of isotropic damage on the infinitesimal changes of nominal stress, consistent differentiation of (3.25) leads to:

$$\delta\boldsymbol{\sigma} = (1 - \omega) \delta\bar{\boldsymbol{\sigma}} - \bar{\boldsymbol{\sigma}} \delta\omega = (1 - \omega) \boldsymbol{\Theta}_{EP} : \delta\boldsymbol{\varepsilon} - \bar{\boldsymbol{\sigma}} \delta\omega \quad (3.93)$$

In order to obtain the perturbation of damage  $\delta\omega$ , linearisation of (3.24) and  $\kappa_d$  in Figure 3.4 allow for the expression:

$$\delta\omega = \frac{dg_d}{d\kappa_d} \delta\tilde{\varepsilon}$$

$$\delta\omega = \frac{1}{x_s} \frac{dg_d}{d\kappa_d} \left[ \Delta\lambda \left( \frac{\partial m_v}{\partial \bar{\sigma}_v} - \frac{m_v}{x_s} \frac{\partial x_s}{\partial \bar{\sigma}_v} \right) \delta\bar{\sigma}_v + \Delta\lambda \left( \frac{\partial m_v}{\partial \bar{\rho}} - \frac{m_v}{x_s} \frac{\partial x_s}{\partial \bar{\rho}} \right) \delta\bar{\rho} + \Delta\lambda \frac{\partial m_v}{\partial \kappa_p} \delta\kappa_p + m_v \delta\lambda \right] \quad (3.94)$$

Since  $\delta\bar{\sigma}_v$ ,  $\delta\bar{\rho}$ ,  $\delta\kappa_p$  and  $\delta\lambda$  can be put as a function of  $\delta\varepsilon$  with (3.83), the second term of the right hand side in (3.93) develops into:

$$\bar{\sigma} \delta\omega = \frac{dg_d}{d\kappa_d} (\bar{\sigma} \otimes \boldsymbol{\eta}) : \delta\varepsilon = \frac{dg_d}{d\kappa_d} \left( \bar{\sigma} \otimes \frac{\partial \tilde{\varepsilon}}{\partial \varepsilon} \right) : \delta\varepsilon \quad (3.95)$$

As with the perturbations in effective stress, this is expressed in  $\mathbf{n}_I$  base at first, and then changed via the spectral matrix. Finally, combining (3.95) and (3.93):

$$\delta\sigma = \left( (1-\omega) \boldsymbol{\Theta}_{EP} - \frac{dg_d}{d\kappa_d} (\bar{\sigma} \otimes \boldsymbol{\eta}) \right) : \delta\varepsilon = \boldsymbol{\Theta}_{EPD} : \delta\varepsilon \quad (3.96)$$

Alternatively, for the case of anisotropic damage, it is (3.29) that needs consistent differentiation, thus leading to:

$$\delta\sigma = \tilde{\boldsymbol{\omega}}^2 \cdot \delta\bar{\sigma} + \delta\tilde{\boldsymbol{\omega}}^2 \cdot \bar{\sigma} = \tilde{\boldsymbol{\omega}}^2 \cdot \boldsymbol{\Theta}_{EP} : \delta\varepsilon - \delta\omega \cdot \bar{\sigma} \quad (3.97)$$

with the second order tensors  $\tilde{\boldsymbol{\omega}}$  and  $\boldsymbol{\omega}$  related in (3.28), and expressed initially in their principal base. Recalling (3.45), along with the same formal disquisitions that led to (3.78)-(3.79), allows to rewrite the perturbation in the damage tensor as:

$$\delta\omega_{JJ} = \delta\omega_J = \frac{g'_d \varepsilon_{P,JJ}^2}{\boldsymbol{\delta} : \boldsymbol{\varepsilon}_P^2} \boldsymbol{\eta} : \delta\varepsilon \quad (3.98)$$

$$\delta\omega_{IJ} \Big|_{I \neq J} = \frac{\omega_I - \omega_J}{2(\varepsilon_{eI}^{tr} - \varepsilon_{eJ}^{tr})} \delta\gamma_{IJ} \quad (3.99)$$

resorting to formally identical provisions as in (3.80) in case of coincidence of two principal trial strain values. These only necessitate a damage deviatoric radius defined as with stresses and strains:

$$\rho_\omega = \sqrt{\mathbf{s}_\omega : \mathbf{s}_\omega} \quad (3.100)$$

where  $\mathbf{s}_\omega$  is the deviatoric part of the damage tensor. Substitution of (3.98) and (3.99) in (3.97) leads to a linear system generically expressed as:

$$\delta\sigma = \tilde{\omega}^2 \cdot \Theta_{EP} : \delta\epsilon - \Theta_D : \delta\epsilon = \Theta_{EPD} : \delta\epsilon \quad (3.101)$$

conveniently transformed to Cartesian base via the spectral matrix.

From the general expressions (3.96) and (3.101), it is possible to assess the special case of apex return, both fixed and iterative, as discussed in Section 3.3. If the hardening process is still ongoing, and considering that a stress-return leading to the apex implies  $\bar{\rho} = 0$  and  $\delta\bar{\rho} = 0$  (as an infinitesimal change in the trial stress coordinates will not change the stress-return type), substitution of these conditions in (3.78) and (3.79) shows that:

$$\delta\bar{\sigma}_1 = \delta\bar{\sigma}_2 = \delta\bar{\sigma}_3 = \delta\bar{\sigma}_V \quad (3.102)$$

i.e. there is only an infinitesimal change in the volumetric component of effective stress which can be obtained from (3.83) by previous substitution of the Jacobian (3.42). Moreover, since continuing hardening can only occur for  $\kappa_p < 1$  and, by virtue of (3.21), for  $\kappa_d = 0$ , it then follows that  $\omega = 0$  and  $\delta\omega = 0$  in the isotropic case, or  $\tilde{\omega} = \mathbf{0}$  and  $\delta\omega = \mathbf{0}$  in the anisotropic case, leading to:

$$\begin{aligned} \delta\sigma_{apex_i} &= \left( (1-0)\Theta_{EP}^{apex_i} - \mathbf{0} \right) : \delta\epsilon = \Theta_{EPD}^{apex_i} : \delta\epsilon, \text{ isotropic} \\ \delta\sigma_{apex_i} &= \left( \tilde{\delta}^2 \cdot \Theta_{EP}^{apex_i} - \mathbf{0} \right) : \delta\epsilon = \Theta_{EPD}^{apex_i} : \delta\epsilon, \text{ anisotropic} \end{aligned} \quad (3.103)$$

after substitution of  $\delta\bar{\sigma}_V$  in (3.78) and changing base appropriately.

If, on the other hand, hardening has reached completion, then  $\delta\bar{\sigma} = \mathbf{0}$  as any perturbation  $\delta\epsilon$  leads to the same returned apex, and consequently  $\Theta_{EP}^{apex_d} = \mathbf{0}$ . Infinitesimal changes in nominal stress stem solely from the damage part and hence:

$$\begin{aligned} \delta\sigma_{apex_d} &= \left( \mathbf{0} - \frac{d\mathbf{g}_d}{d\kappa_d} (\bar{\sigma} \otimes \eta)_{apex_d} \right) : \delta\epsilon = \Theta_{EPD}^{apex_d} : \delta\epsilon, \text{ isotropic} \\ \delta\sigma_{apex_d} &= (\mathbf{0} - \Theta_D) : \delta\epsilon = \Theta_{EPD}^{apex_d} : \delta\epsilon, \text{ anisotropic} \end{aligned} \quad (3.104)$$

after retrieval of  $\delta\lambda$  from (3.83) and changing base appropriately.

Regardless of the type of apex return, the aforementioned steps can be followed even for the limit cases  $\bar{\theta} = 0$  and  $\bar{\theta} = \pi/3$ , by resorting to (3.92) instead of (3.82). Should an incremental step lead to elastic unloading after triggering of damage, then  $\delta\omega = 0$  or  $\delta\omega = \mathbf{0}$  without change of the accumulated damage or plastic strains:

$$\begin{aligned}\delta\sigma_{unload} &= ((1-\omega)\mathbf{D}_e - \mathbf{0}) : \delta\boldsymbol{\varepsilon} = \boldsymbol{\Theta}_{EPD}^{unload} : \delta\boldsymbol{\varepsilon}, \text{ isotropic} \\ \delta\sigma_{unload} &= (\tilde{\mathbf{w}}^2 \cdot \mathbf{D}_e - \mathbf{0}) : \delta\boldsymbol{\varepsilon} = \boldsymbol{\Theta}_{EPD}^{unload} : \delta\boldsymbol{\varepsilon}, \text{ anisotropic}\end{aligned}\tag{3.105}$$

As commented in Section 3.3.2, the calculation of  $\boldsymbol{\Theta}$  consistent with a sub-incrementation scheme requires updating at every sub-incremental step. That is, linearisations must be made consistently with every sub-incremental stress evaluation, as a perturbation in the finite strain increment entails stress perturbations at every sub-incremental level. This not only makes the corresponding formulation more cumbersome but considerably increases the associated computational demand. Hence, since the novel robustness measures introduced in Section 3.3 enable a high convergence ratio without resorting to sub-incrementation, they also favour performance.

For illustration, however, although such a scheme is not applied in the present work, the derivation of the algorithmic stiffness from the reduced system of simultaneous equations (3.31) – as opposed to the full formulation, as in Valentini and Hofstetter (2013) - for isotropic damage is illustratively included in Appendix A.

### 3.5 CDPM localisation tensor and directional properties

Strain localisation analysis provides the formal framework in which to articulate the condition for a jump across surfaces delimiting a narrow localisation band to occur in the strain field, whilst keeping a continuous displacement field (also known as weak discontinuity). The theory behind this condition and the development for plasticity and damage has been extensively treated by Rudnicki and Rice (1975), and Rizzi *et al.* (1995) respectively. The current section provides only a brief summary of the steps leading to the localisation condition, strongly based on Jirásek (2014), and investigates subsequently into its application to the isotropic damage version of the CDPM.

Localisation analysis, in its classical form, refers to a single point belonging to the surface where strain discontinuity is incipient. At that stage, just before onset of localisation, only the strain- and stress *rate* fields are discontinuous across that surface. By constraining these rate jumps via the traction continuity condition:

$$\mathbf{n} \cdot \dot{\boldsymbol{\sigma}}^+ = \mathbf{n} \cdot \dot{\boldsymbol{\sigma}}^- \tag{3.106}$$

and the displacement continuity condition:

$$\dot{\boldsymbol{\varepsilon}}^+ = \dot{\boldsymbol{\varepsilon}}^- + \dot{\boldsymbol{\varepsilon}}(\mathbf{p} \otimes \mathbf{n})_{sym} \quad (3.107)$$

respectively, the rate jumps remain bounded, provided small-strain theory is applicable. The superscripts + and – denote the limit to which  $\dot{\boldsymbol{\sigma}}$  and  $\dot{\boldsymbol{\varepsilon}}$  tend from different sides of the discontinuity surface,  $\mathbf{n}$  is the unit normal to the discontinuity surface at the point of interest,  $\dot{\boldsymbol{\varepsilon}}$  is the magnitude of the vector containing all rate jump components and  $\mathbf{p}$  is the so-called polarisation vector, the unit vector associated to  $\dot{\boldsymbol{\varepsilon}}$ . Combination of (3.106) and (3.107) with the rate form of the stress-strain equations, along with the assumption that the material behaves identically at both sides of the discontinuity surface ( $\mathbf{D}^+ = \mathbf{D}^- = \mathbf{D}$ ) when the onset of localisation is incipient, leads to:

$$(\mathbf{n} \cdot \mathbf{D} \cdot \mathbf{n}) \cdot \mathbf{p} = 0 \quad (3.108)$$

where  $\mathbf{D}$  is the tangent stiffness tensor. By introducing the second order tensor:

$$\mathbf{Q} = \mathbf{n} \cdot \mathbf{D} \cdot \mathbf{n} \quad (3.109)$$

the localisation condition (3.108) further simplifies to:

$$\mathbf{Q} \cdot \mathbf{p} = 0 \quad (3.110)$$

$\mathbf{Q}$  is typically referred to as acoustic tensor, which stems from the original study of wave propagation inside continua: the eigenvalues of  $\mathbf{Q}$  are proportional to the squares of the speeds of waves propagating in direction  $\mathbf{n}$  (Jirásek, 2014). It also justifies the name of  $\mathbf{p}$ , as it determines the type of wave. In this case, under the condition of incipient weak discontinuity (3.110),  $\mathbf{p}$  represents the eigenvector associated to a zero eigenvalue of  $\mathbf{Q}$  (or, in the classical context, the polarisation vector of a stationary wave). Thus, the final and most compact expression of the localisation condition is:

$$\det(\mathbf{Q}) = 0 \quad (3.111)$$

with  $\mathbf{Q}$  being generalised in this context to be called localisation tensor. The direction  $\mathbf{n}$  for which condition (3.111) is fulfilled represents the normal of a potential localisation band orientation, only valid in the local vicinity of the point considered. Coalescing into a macro band requires condition (3.111) to be satisfied in a sufficient number of points. However, singularity of the localisation tensor is a good indicator of potential discontinuities. The failure mode is given by the polarisation vector as follows:

$$\begin{aligned} \mathbf{n} \cdot \mathbf{p} &= 1, & \text{mode I (tensile splitting)} \\ \mathbf{n} \cdot \mathbf{p} &= 0, & \text{mode II (shear slip)} \\ 0 < \mathbf{n} \cdot \mathbf{p} < 1, & \text{mixed mode} \end{aligned} \quad (3.112)$$

The mathematical definition of the localisation condition is based on differential rate equations, which should theoretically entail the usage of the material tangential stiffness  $\mathbf{D}$  (Section 3.4). However, any actual analysis based on (pseudo)time discretisation resorts to finite increments, and therefore it is arguably more consistent to consider  $\mathbf{\Theta}_{EPD}$  as the operator entering (3.109). By doing so, and after some algebraic elaborations, the CDPM localisation tensor is obtained as:

$$\mathbf{Q}_{EPD} = (1 - \omega) \mathbf{n} \cdot \mathbf{\Theta}_{EP} \cdot \mathbf{n} - g'(\mathbf{n} \cdot \bar{\boldsymbol{\sigma}}) \otimes (\boldsymbol{\eta} \cdot \mathbf{n}) \quad (3.113)$$

where a reasonable simplification of  $\mathbf{\Theta}_{EP}$  to use in (3.113) can be obtained as:

$$\mathbf{\Theta}_{EP} = \boldsymbol{\Xi} - \frac{1}{h_{\boldsymbol{\varepsilon}}} \left[ \boldsymbol{\Xi} : \frac{\partial \mathbf{g}_p}{\partial \bar{\boldsymbol{\sigma}}} \otimes \frac{\partial f_p}{\partial \bar{\boldsymbol{\sigma}}} : \boldsymbol{\Xi} \right] \quad (3.114)$$

by means of the pseudo-elastic stiffness tensor:

$$\boldsymbol{\Xi} = \left[ \mathbf{I} - \Delta \lambda \mathbf{C} : \frac{\partial \mathbf{m}}{\partial \bar{\boldsymbol{\sigma}}} \right]^{-1} : \mathbf{C} \quad (3.115)$$

and the following remaining entities:

$$h_{\boldsymbol{\varepsilon}} = \frac{\partial f_p}{\partial \bar{\boldsymbol{\sigma}}} : \boldsymbol{\Xi} : \frac{\partial \mathbf{g}_p}{\partial \bar{\boldsymbol{\sigma}}} + k_p H \quad (3.116)$$

$$H = - \frac{\partial f_p}{\partial \kappa_p} \quad (3.117)$$

In (3.115),  $\mathbf{I}$  stands for the unit fourth order tensor and  $\mathbf{C}$  for the elastic compliance tensor.

In order to assess the directional properties of the CDPM localisation tensor as obtained here, and due to the purely local character of the localisation condition allowing for its point wise monitoring, a simple numerical test is performed, following Leroy and Ortiz (1989) and Pivonka and Willam (2003). This test is based on a single finite element under compression. Originally, the formulation assumed the element to be a 2-dimensional linear quadrilateral under plane-strain conditions. In the present context, the element is a quadratic hexahedron appropriately scaled to match the original geometry (1m x 1m x 0.1m), with equivalent boundary conditions (depicted in Figure 3.25).

In this case, the orientation of the localisation band can be described solely by means of the angle  $\gamma$  or the angle  $\varphi$  (both measured from X in the XZ plane), depending on reference

being made to the normal  $\mathbf{n}$  or to the band itself, respectively (Figure 3.25a). Consequently, condition (3.111) can be checked against the range of either angle at every incremental step. Figure 3.25b shows the evolution of the normalised determinant of the CDPM localisation tensor against angle  $\varphi$ , using as normalising measure the determinant of the elastic acoustic tensor  $\mathbf{Q}_e = \mathbf{n} \cdot \mathbf{D}_e \cdot \mathbf{n}$ :

$$\det_n(\mathbf{Q}_{EPD}(\mathbf{n})) = \frac{\det(\mathbf{Q}_{EPD}(\mathbf{n}))}{\det(\mathbf{Q}_e(\mathbf{n}))} \quad (3.118)$$

with

$$\mathbf{n} = \begin{Bmatrix} \cos \varphi \\ 0 \\ \sin \varphi \end{Bmatrix} \quad (3.119)$$

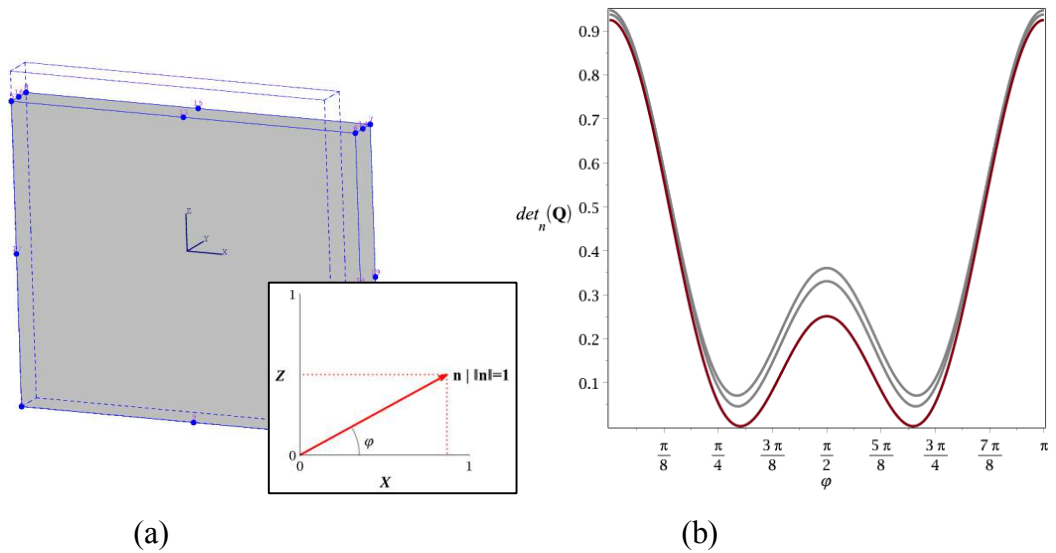


Figure 3.25: (a) Single 20-noded element for the compression test; deflection magnified by a factor of 20 at onset of localisation (b) Evolution of normalised determinant  $\det_n(\mathbf{Q})$  vs. inclination of the band  $\varphi$ ;  $\kappa_p = 0.30$  (grey),  $0.35$  (grey) and  $0.51$  (red)

The inclination corresponding to initial singularity of  $\mathbf{Q}_{EPD}$  is  $\varphi \approx 53^\circ$  (shown in Figure 3.25b along with the symmetrical solution), which is in good agreement with previous results. However, whilst Pivonka and Willam (2003) resorted to the Extended Leon Model (Etse and Willam, 1994), with Lode's angle entering the definition of plastic potential and a significant sensitivity of  $\varphi$  to the eccentricity (3.7), directional accuracy is achieved here with a constant eccentricity and radial returns. The latter poses a significant advantage in sight of the

numerical robustness decrease if the stress-return does not follow a constant meridian plane, particularly for eccentricity values below the lower bound  $e = 0.665$  proposed by Etse (1992). Additionally, the only way to ensure radial returns in the Extended Leon Model is by enforcing the eccentricity to be  $e = 1$ , which in turn shifts the result to the characteristic value of  $J_2$  plasticity ( $\varphi \approx 45^\circ$ ), as clearly shown in Pivonka and Willam (2003).

Formally following the original elaborations in Rice (1976), it is possible to derive an explicit expression for the localisation condition in terms of one of the intervening CDPM variables should the localisation tensor become singular before onset of damage (as is the case in Figure 3.25b). The resulting localisation condition relates to a critical value of  $(k_p H)$  over all possible orientations of  $\mathbf{n}$ , only below which localisation is possible:

$$(k_p H)_{\text{cr}} = \max \left[ \mathbf{a}_{\Xi} \cdot \mathbf{Q}_{\Xi}^{-1} \cdot \mathbf{b}_{\Xi} - \frac{\partial f_p}{\partial \bar{\sigma}} : \Xi : \frac{\partial g_p}{\partial \bar{\sigma}} \right] \quad (3.120)$$

Illustratively, Figure 3.26 shows  $(k_p H)$  for the reference state corresponding to the onset of localisation, depicted with a red curve in Figure 3.25b:

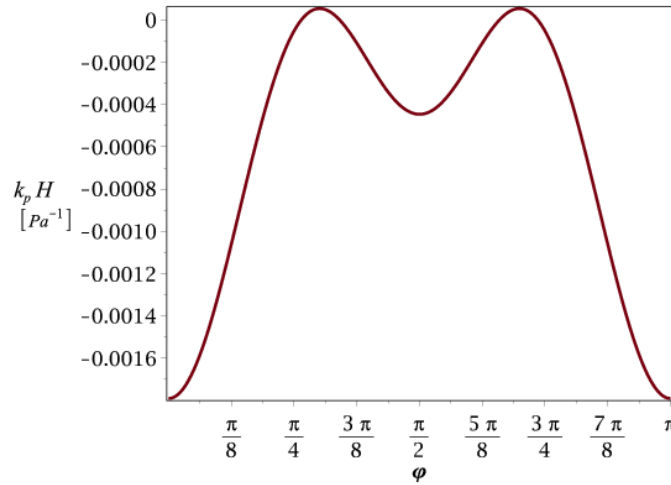


Figure 3.26: Generalised plastic modulus  $(k_p H)$  at onset of localisation in a given sample point of the single 20-noded element

As expected, the values of  $\varphi$  for which the localisation tensor becomes singular also define the orientations with a critical generalised plastic modulus  $(k_p H)$ . It is noteworthy that such critical value is positive, i.e. that localisation into a finite band occurs during hardening and

before the onset of damage. This is a direct consequence of non-associativity (or ‘lack of normality’) in the plastic flow, as noted in Rudnicki and Rice (1975).

The main outcome from localisation analysis to the isotropic damage version of the CDPM is thus twofold: the numerical test on a single element indicates that good directional properties can be expected from the model despite the absence of Lode’s angle in the definition of the plastic potential, and the non-associativity of the plastic flow rule may potentially entail the localisation onset to take place already during plastic hardening. In light of these features, it is decided to investigate if resorting to localisation analysis can alleviate the mesh-induced directional bias affecting Finite Element simulations. This is done by using  $\mathbf{n}$ ,  $\mathbf{p}$  and their relative orientation as assessed in (3.112) to redefine the spectral matrix, as the scalar product of  $\mathbf{n}$  and  $\mathbf{p}$  establishes whether or not applying rotations is necessary to have them aligned with principal directions. The assessment of localisation analysis on directional bias applied to a benchmark simulation is discussed in Chapter 5.

### 3.6 Regularisation and fracture energy

From a mathematical perspective, localisation, as elucidated in Section 3.5 and enabled by equation (3.111), corresponds to a loss of ellipticity of the governing system of differential equations (equilibrium, kinematic and constitutive) in static or quasi-static analysis of rate-independent materials, whereas for dynamic analysis the differential equations lose their hyperbolic character. Either way, such loss mathematically allows for potential discontinuities in the solution and entails the associated global problem (boundary value problem for statics and initial value problem for dynamics) losing its well-posedness. Consequently, the number of independent solutions becomes unbounded and, dimensionally, the need for an internal length scale arises. In its absence, the width of the localisation band cannot be numerically resolved and hence objectivity of numerical analysis is lost, as such bandwidth can decrease arbitrarily with mesh refinement. In the limit, full localisation would happen in a zero-volume band, therefore dissipating no energy, which is physically unsound (de Borst *et al.*, 2012).

One way to address the described issue is resorting to localisation limiters, either by incorporating higher-order gradients of the internal variables into the constitutive model or via an integral non-local continuum formulation (Jirásek and Bazant, 2002). The former can

be found elaborated in Pamin (2005) whereas the latter has already been applied to the damage part of a later version of the CDPM by Grassl *et al.* (2013). Both approaches, however, imply a considerable computational cost, particularly when calculating the algorithmic tangential stiffness  $\Theta$ . An alternative to localisation limiters that allows maintaining a local continuum formulation is the so-called mesh-adjusted softening modulus technique or crack band approach. Based on the work of Bazant and Oh (1983), amongst others (Rots *et al.*, 1985; de Borst, 1986; Lubliner *et al.*, 1989), this approach postulates the energy represented by the area under the traction-separation law to be a material property. This property corresponds to the energy required to create a unit area of the completely developed crack surface, i.e. the fracture energy  $G_f$ . Adjustment of the stress-inelastic strain relation such that the enclosed area (i.e. energy per unit volume or specific fracture energy  $g_f$ ) satisfy:

$$g_f = \frac{G_f}{h} \quad (3.121)$$

allows for a reasonable objectivity. In (3.121),  $h$  is an estimator of the numerically resolved crack bandwidth, only available *a posteriori*, with the level of achieved objectivity being linked to the accuracy of  $h$ . Moreover,  $h$  responds to the dimensional need for an internal length scale upon localisation. Noting that under uniaxial tension the internal strain-like variables  $\kappa_p$  and  $\kappa_d$  evolve identically with a shift of 1, and that the curve governed by (3.24) corresponds to a uniaxial nominal stress-uniaxial plastic strain curve, as shown in Figure 3.27, it follows that the parameter controlling the adjustment (via the slope) is  $\varepsilon_f$ , in turn dependent on the crack bandwidth estimator  $h$ .

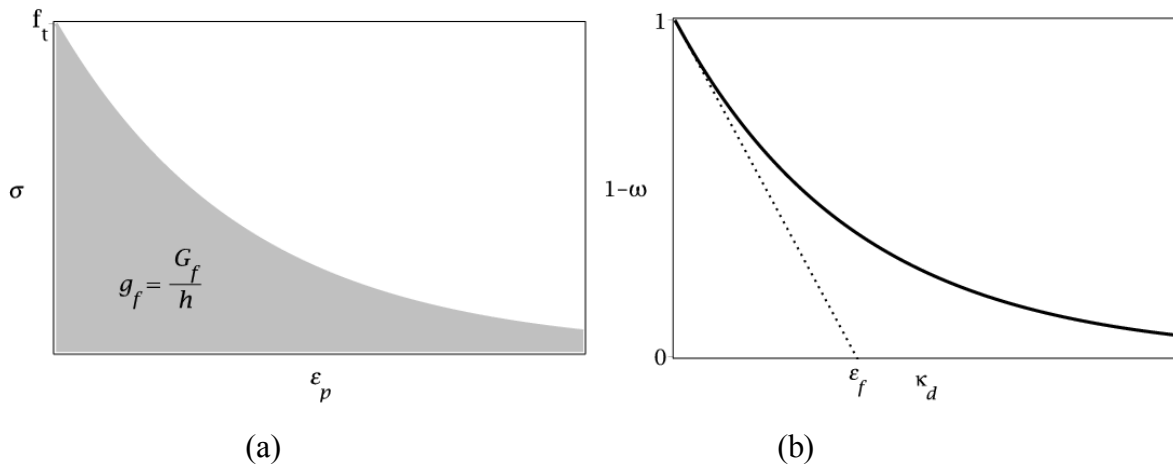


Figure 3.27: (a) Nominal stress-plastic strain under uniaxial tension (b) Complementary damage curve as given by (3.24)

The consistent derivation of  $h$  as a function of the element geometric characteristics and orientation of the crack or localisation band stems originally from Oliver (1989), and has later been reviewed and enhanced by Slobbe *et al.* (2013) and Govindjee *et al.* (1995) for three-dimensional elements. According to the latter, the bandwidth estimator can be obtained as:

$$h = \left( \left[ \sum_{i=1}^{n_c} \frac{\partial N_i(\xi)}{\partial \xi} \tau_i \right] \cdot \frac{\partial \xi}{\partial \mathbf{x}} \cdot \mathbf{n} \right)^{-1} \quad (3.122)$$

where  $n_c$  is the number of corner nodes,  $N_i$  stands for the shape function associated with corner node  $i$  of a linear element of  $n_c$  nodes (since for higher order elements, the total number of nodes  $n_N \neq n_c$ ),  $\frac{\partial \xi}{\partial \mathbf{x}}$  is the inverted transpose of the transformation Jacobian between element intrinsic ( $\xi$ ) and Cartesian ( $\mathbf{x}$ ) coordinates,  $\mathbf{n}$  is the unit normal to the band and  $\tau_i$  are nodal values calculated as:

$$\tau_i = \frac{(\mathbf{x}_i - \mathbf{x}_c) \cdot \mathbf{n} - \tau_{\min}}{\tau_{\max} - \tau_{\min}} \quad (3.123)$$

with:

$$\begin{aligned} \tau_{\min} &= \min_{i=1, n_c} \{(\mathbf{x}_i - \mathbf{x}_c) \cdot \mathbf{n}\} \\ \tau_{\max} &= \max_{i=1, n_c} \{(\mathbf{x}_i - \mathbf{x}_c) \cdot \mathbf{n}\} \end{aligned}$$

and  $\mathbf{x}_c$  as the coordinates of the element interpolation centroid. Function  $\tau$  is a continuous generalisation of the binary crack indicator function  $\phi$  originally introduced by Oliver (1989). Whilst  $\phi$  could only assign the values 0 or 1 to (corner) nodes *behind* or *in front* of the band respectively (the *forward* direction sense being given by  $\mathbf{n}$ ),  $\tau$  allows for a continuous transition between 0 and 1. In any case, the crack indicator function is interpolated across the band by means of the same shape functions entering (3.122), precisely derived initially from the inverse of the derivative of  $\tau$  in the direction given by  $\mathbf{n}$ . As indicated by Slobbe (2015), replacing of  $\phi$  by  $\tau$  ensures a continuous dependence of  $h$  on the band orientation. Also, it can be shown that, in essence, Govindjee's formulation of the bandwidth estimator pertains to projection methods, whereby  $h$  would correspond to the distance from the node(s) attaining  $\tau_{\min}$  to the node(s) attaining  $\tau_{\max}$  along direction  $\mathbf{n}$ . This in turn implies independence of  $h$  with respect to the specific position of the sample point in consideration.

In Oliver (1989), it is specified that  $\mathbf{n}$  should be obtained via localisation analysis, which could be done following the provisions of Section 3.5. In the absence of this analysis, however, it is shown in Jirásek and Horák (2010) that for rotating crack models localisation can be triggered along with the onset of cracking, with  $\mathbf{n}$  being coincident with the normal to the crack. Since the underlying formulation in the CDPM is that of a smeared rotating (coaxial) crack model, and it is shown in Section 3.5 that onset of localisation can coincide or even precede damage, it is considered justified to assume  $\mathbf{n}$  as the direction of the first principal strain in the version of the model not resorting to localisation analysis. By doing so, an additional relation between  $h$  and principal directions of strain is introduced that must be accounted for in the calculation of the algorithmic stiffness presented in Section 3.4 for consistency. The necessary elaborations to obtain this additional term for the case of isotropic damage can be found in Appendix B.

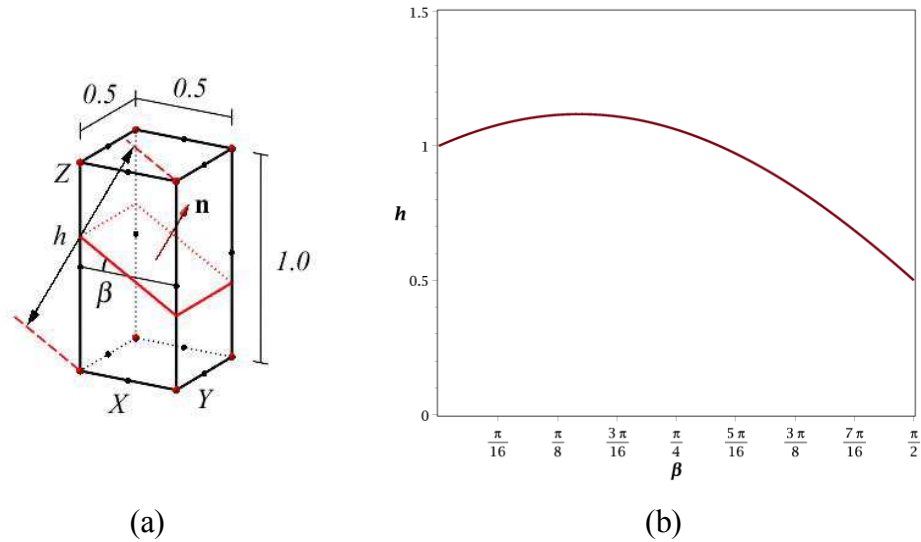


Figure 3.28: (a) Hexahedral element with crack band passing through the centroid  
(b) Bandwidth estimator distribution with rotating  $\mathbf{n}$  in the XZ plane

Following Slobbe *et al.* (2013), Govindjee's formulation is assessed here for a three-dimensional hexahedral element, with geometry as shown in Figure 3.28a. Considering the unit normal  $\mathbf{n}$  to be contained in the XZ plane, and the sample point to be in the element interpolation centroid, the orientation of the band and consequently the bandwidth estimator are exclusively functions of angle  $\beta$ . Figure 3.28b shows the resulting continuous distribution of  $h$  with varying  $\beta$ .

For a more generic orientation of the unit normal, a second rotation  $\varpi$  is needed (Figure 3.30a). Resorting to a spherical coordinate system as the one depicted in Figure 3.29, the distribution of  $h$  generalises into a surface, as shown in Figure 3.30b. The curve highlighted in red corresponds to the particular case that  $\theta_1 = 0$  (or  $\theta_1 = \pi/2$ ), hence reverting back to Figure 3.28b.

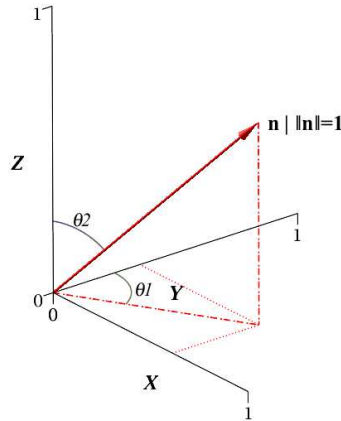


Figure 3.29: Reference spherical coordinate system

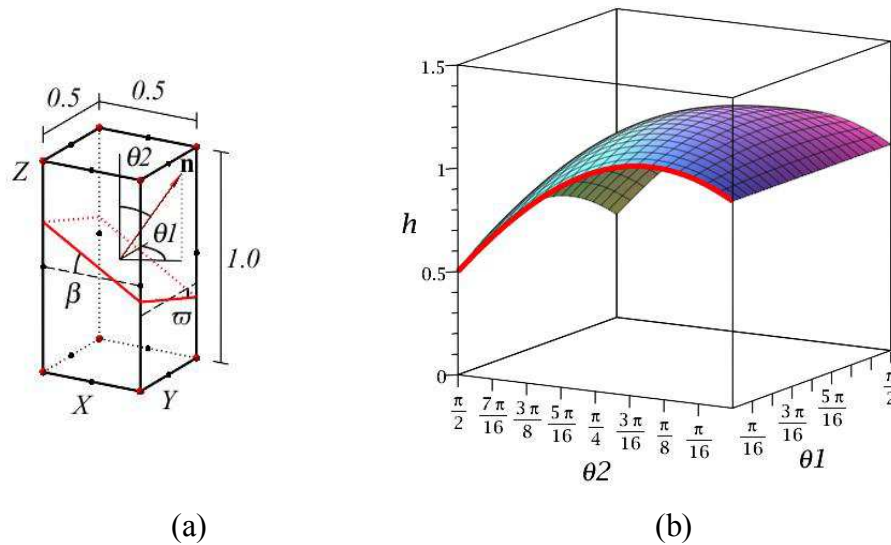
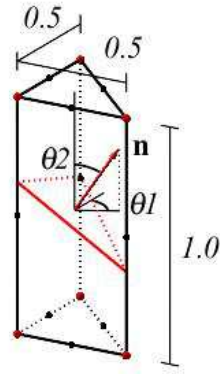
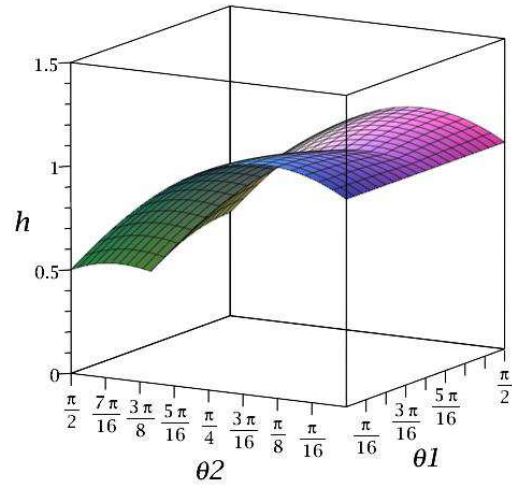


Figure 3.30: (a) Hexahedral element with generically oriented crack band passing through the centroid (b) Bandwidth estimator spatial distribution

Maintaining the auxiliary spherical system and changing the type of element from an hexahedron to a pentahedron (wedge), a tetrahedron and a pyramid gives rise to the spatial distribution of  $h$  shown in Figures 3.31, 3.32 and 3.33, respectively.

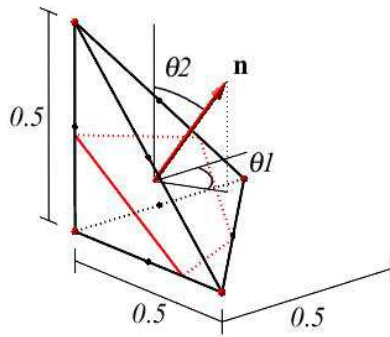


(a)

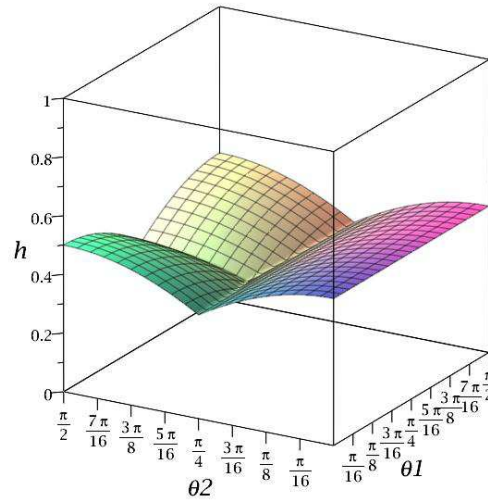


(b)

Figure 3.31: (a) Wedge element with generically oriented crack band passing through the centroid (b) Bandwidth estimator spatial distribution



(a)



(b)

Figure 3.32: (a) Tetrahedral element with generically oriented crack band passing through the centroid (b) Bandwidth estimator spatial distribution

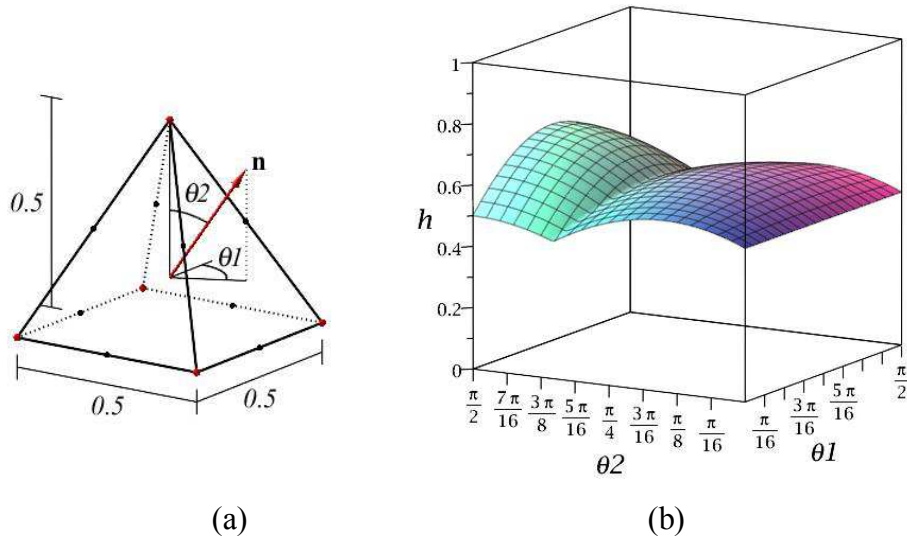


Figure 3.33: (a) Pyramid element with generically oriented crack band passing through the centroid (b) Bandwidth estimator spatial distribution

Recalling Figure 3.27 and the geometric meaning of  $\varepsilon_f$ , and defining  $\varepsilon_0 = \bar{f}_t / E$  as the (equivalent) uniaxial strain at peak stress, the relation between the adjustment parameter and the crack bandwidth estimator can be established. For clarity, the stress-strain diagram of Figure 3.27 is extended in Figure 3.34a to refer to total strain, along with the geometric representation of  $\varepsilon_0$ .

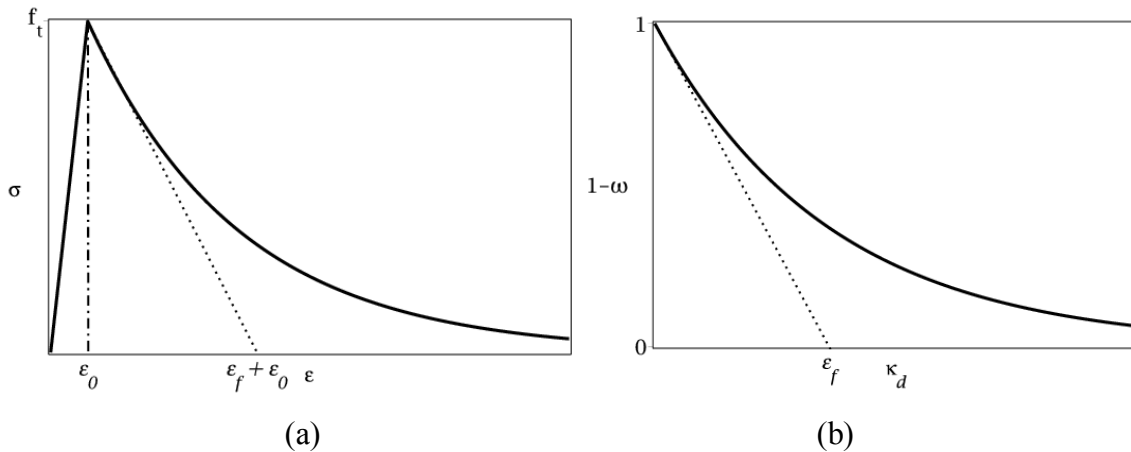


Figure 3.34: (a) Nominal stress-total strain under uniaxial tension, (b) Complementary damage curve as given by (3.24)

Integration of the curve depicted in Figure 3.34a represents precisely the specific fracture energy (3.121):

$$\frac{G_f}{h} = \int_0^{\infty} \sigma(\varepsilon) d\varepsilon \quad (3.124)$$

Substitution in (3.124) of the exponential law given by (3.24) leads, after some rearrangements, to:

$$\varepsilon_f = -\frac{\varepsilon_0}{2} + \frac{G_f}{h f_t} \quad (3.125)$$

As can be seen from Figure 3.27 and equation (3.125), excessive values of  $h$  may cause the adjustment parameter to fall below zero (or the total equivalent strain to fall below  $\varepsilon_0$ ), which would entail a snap-back in the material response in the sample point under consideration. To avoid this undesired (and physically inadmissible) feature, the restriction  $\varepsilon_f \geq 0$  must be imposed, which in turn leads to:

$$h \leq \frac{2G_f E}{f_t^2} = h_{cr} \quad (3.126)$$

Should restriction (3.126) not be satisfied by the appropriate bandwidth estimator (3.122), then the critical threshold value  $h = h_{cr}$  must be adopted. It should be noted, however, that although a reasonable objectivity with regards to the mesh size is achieved with this approach, there is still an inherent mesh induced directional bias at the core of smeared softening formulation. This feature is noted in the numerical simulations of Chapter 5. Although localisation limiters seem to alleviate the directional bias, its consistent treatment is still the subject of research (e.g. Slobbe (2015)).

Despite its ease of implementation, the crack band approach has the drawback of requiring the calculation of the bandwidth estimator for each element at every iterative step at the global level, which hinders performance and may seem counterproductive with respect to the various measures adopted hitherto. Also, since the final direction of the macro-crack (or band of damage in this case) may vary during the process of its formation,  $h$  (and hence  $\varepsilon_f$ ) does not have to remain constant for the same stress-strain curve, potentially affecting its shape. If the mesh areas where damage propagation is expected to occur are not significantly irregular, it is considered as computationally more efficient to predefine  $h$  and leave it as a fixed parameter. It would then have the character of a representative element size, dependent on the *a priori* estimated relative orientation of the element with respect to the expected final

damage band and the expected level of localisation within the element. The latter factor is of relevance, since for quadratic elements (with full or reduced integration scheme) it is possible for the band to localise into a subset of Gauss points. To accommodate this possibility, a factor  $\gamma$  should affect the first estimation of parameter  $h$  solely based on orientation, with the range of  $\gamma$  for most subset options in all elements typically ranging between 0.5 and 0.7. With the considerations of computational performance in mind, it is decided to adopt  $h$  as a fixed parameter instead of an internal variable in the final implemented version of the model. However, a comparison between the two approaches applied to a numerical example is presented and discussed in Chapter 5.

### 3.7 Conclusions

The present chapter introduces the CDPM and elaborates on its algorithmic structure and implementation strategy. Focus is centred on the main novel enhancements involving the subdivision of the effective stress space to trigger different types of stress-returns, alongside a sequence of *a priori* and *a posteriori* checks and a line search scheme, which prove to significantly contribute to the numerical robustness of the implemented model.

The underlying reason for previous robustness issues is shown to be the potential singularity of the Jacobian at either the initial trial stress state or an intermediate iterative stress state. Whilst a reduction of the rank of simultaneous equations by decoupling the internal strain-like plastic variable proves thoroughly advantageous in the former case, the latter necessitates the proposed line search scheme to avoid Jacobian singularity or even convergence to inadmissible stress states.

Upon numerical testing of the implemented module, the increase in robustness is confirmed by achieving a full convergence ratio, which previous works fail to attain. The proposed modification to reconcile the discontinuity of returned stress states close to or strictly on the hydrostatic axis, though consistent and more intuitive, implies a decrease in the convergence rate for the numerical test, retaining full convergence ratio nonetheless, and is therefore discarded.

New provisions are presented whilst elaborating the elasto-plastic-damage algorithmic stiffness, in order to accommodate the case of stress-returns along the tensile or compressive

meridian planes, hitherto untreated. The resulting consistent derivation of this operator allows for resorting to a full Newton scheme for the global boundary value problem once the material model is implemented in the nonlinear Finite Element software ADAPTIC (Izzuddin, 1991).

By means of localisation analysis on the CDPM, the good directional properties of the model are confirmed, and its efficiency and robustness are corroborated by the results of a single element test, achieved despite the invariance of Lode's angle during stress return and a constant eccentricity parameter.

The original damage part of the CDPM is isotropic, and is extended in this chapter to anisotropic formulation, shifting the character of internal variable controlling the softening process to the trace of the damage tensor. Since damage is evaluated explicitly, this generalisation does not alter numerical robustness, and the assessment and comparison between anisotropic and isotropic damage can be found in Chapters 5-6.

A suitable regularisation formulation via the crack band approach is reviewed and elaborated for the quadratic element types used for the simulations in subsequent chapters, although the computational convenience of a fixed damage bandwidth parameter is justified. A comparison backing this approach is presented in one of the simulations in Chapter 5.

# CHAPTER 4

## Modelling of reinforcement

### 4.1 Introduction

The concrete material model (CDPM) introduced and elaborated in Chapter 3 suffices to capture the response of plain concrete under generic three-dimensional stress states. However, incorporation of steel reinforcement bars changes the behaviour of the resulting composite material. The brittleness displayed by plain concrete under predominantly tensile states can be changed to a more ductile response in reinforced concrete, stemming from the contribution of the bars, either elastically or by plastic yielding.

In view of the above, the material modelling of reinforcement must be made consistent with CDPM. To this end, the selected embedded model is presented in Section 4.2 from the range of the most widely used types, with due justification. Sections 4.3.1 to 4.3.4 elaborate the algorithmic treatment of a given bar, focusing on the proposed search and tracking algorithms.

Once all bars are located and tracked, their contribution to concrete elements in terms of stiffness matrix and nodal force vector is obtained in accordance with Section 4.4.

The implemented model is verified in Section 4.5 by means of a control test on a single element model. Validation against experiments can be found in the numerical examples of Chapter 5.

## 4.2 Reinforcement models

When resorting to numerical models for the simulation of reinforcement within reinforced concrete structures, three main approaches can be distinguished: smeared, discrete and embedded, all of which are schematically shown in Figure 4.1.

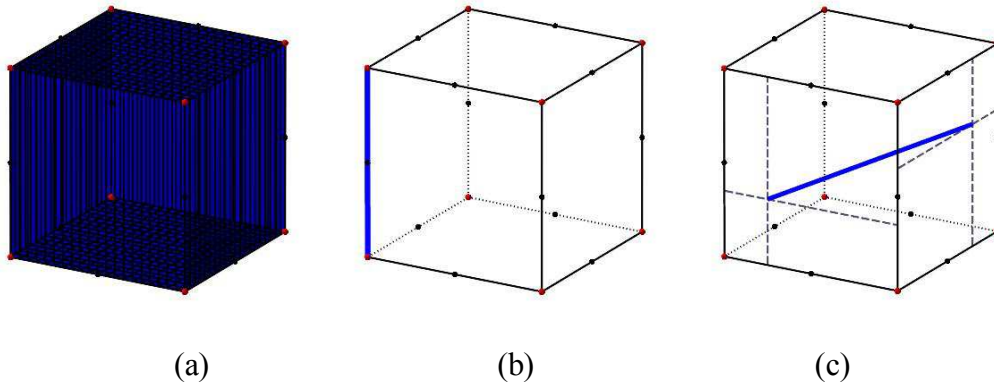


Figure 4.1: Different models for an individual reinforcement bar in a 20-noded hexahedral concrete element (a) smeared (b) discrete (c) embedded

In the smeared approach, steel bars (either individually or by layer) are uniformly distributed across the concrete parent element representing the bulk. This is particularly suitable for reinforcement arrangements where the bars are tightly spaced along structural members of the same dimensional character as the bar layers.

In the discrete approach, each bar is modelled by means of one-dimensional axial elements, whereby the bar nodes are superimposed to those of the concrete parent element, thus following an edge of the latter. Consequently, the spatial orientation of the resulting concrete mesh is guided by the reinforcement arrangement rather than by stress considerations.

The embedded approach, ultimately the reinforcement model adopted in this work, maintains the individual representation of each bar. However, the orientation becomes independent of the concrete parent element edges, as a bar is modelled with the same element type, element order and nodes as the concrete element embedding it, and then combined by addition (see Figure 4.2). Since the framework of the present work is that of three-dimensional discretisation of concrete structures of arbitrary shape, the embedded approach is considered the most appropriate.

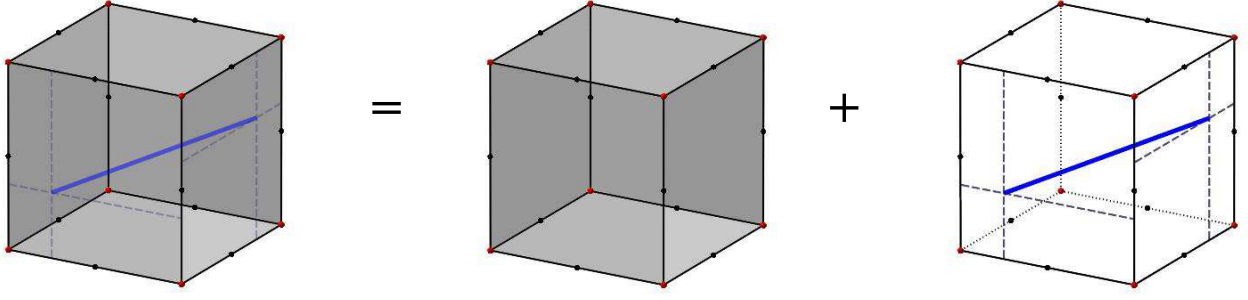


Figure 4.2: Decomposition of a reinforced concrete 20-noded hexahedral element into its two constituents: concrete + embedded bar segment

### 4.3 Algorithmic treatment of bars

Adoption of the embedded approach poses several issues of algorithmic and geometric nature (Hartl, 2002; Huber, 2006). Each physical reinforcement bar (or macro-segment) needs to be located and discretised efficiently inside the three-dimensional concrete mesh. Once located, it is necessary to establish the contributions of the various segments conforming the macro-segment to the subset of parent elements traversed by it, in terms of stiffness matrix and nodal force vector. This in turn means establishing the contributions of each embedded segment to the numerical integration, by means of evaluations at segment Gauss points expressed in terms of parent element coordinates.

All involved steps are schematically presented in Figure 4.3 and individually elaborated in more detail in the sections hereafter.

#### 4.3.1 Search algorithm for macro-segment start point location

In the current framework, only straight macro-segments are considered, as most passive reinforcement arrangements can be fairly represented by open or closed polygonal chains. Hence, a given macro-segment  $b$  can be uniquely described in Cartesian coordinate space by the pair of points  $(\mathbf{P}_S, \mathbf{P}_E)_b$ , where  $\mathbf{P}_S$  and  $\mathbf{P}_E$  stand for start- and end point of  $b$ , respectively. The unit vector connecting these points along the bar axis is  $\mathbf{d}_{SE}$  (Figure 4.4), with:

$$\mathbf{d}_{SE} = \{l_1, m_1, n_1\}^t \quad (4.1)$$

and  $(l_1, m_1, n_1)$  being the direction cosines of the macro-segment.

Given a bar/macro-segment  $(\mathbf{P}_S, \mathbf{P}_E, \mathbf{d}_{SE})_b$  inside a 3D concrete mesh, in general a combination of 20-noded hexahedrons, 10-noded tetrahedrons, 15-noded wedges and 13-noded pyramids:

Identify the parent element  $i$  (or set of feasible candidates) containing  $\mathbf{P}_S$  [  $M$  ] and the relative position of  $\mathbf{P}_S$  with respect to such parent element(s) [  $N_{PE}$  ]

$M \triangleq$  Number of parent elements satisfying

$\left\{ \begin{array}{l} \text{geometric constraint } (R_{CN} \geq R_{PS}) \\ \text{check via Inverse Mapping} \end{array} \right\}$

$N_{PE} = 0 \triangleq \mathbf{P}_S$  is embedded in one parent element

$N_{PE} = 1 \triangleq \mathbf{P}_S$  lies on the face of one or more parent elements

$N_{PE} = 2 \triangleq \mathbf{P}_S$  lies on the edge of one or more parent elements

$N_{PE} = 3 \triangleq \mathbf{P}_S$  lies on a node of one or more parent elements

From  $\mathbf{P}_S$  and along macro-segment  $b$ , proceed to check admissibility of the  $M$  candidates [  $\mathbf{d}_{\xi P} \cdot \bar{\xi}_{k,n}$  ] and select the appropriate reference parent element ( $i$ ) amongst them if necessary, and calculate  $\mathbf{P}_{i,2}$  and  $\mathbf{P}_{i,3}$  via successive linearisations

Dot products  $\mathbf{d}_{\xi P} \cdot \bar{\xi}_{k,n}$  are calculated in the intrinsic coordinate space of the parent element in consideration.

If  $\mathbf{d}_{\xi P} \cdot \bar{\xi}_{k,n} > 0$ , the candidate is deemed inadmissible

Iterative linearising procedure is considered to have converged when  $\mathbf{P}_{i,2}^{PE} = \mathbf{P}_{i,2}^b$  within tolerance

Based on element adjacency considerations, identify the parent element  $j$  (or set of feasible candidates) containing  $\mathbf{P}_{i,2} = \mathbf{P}_{j,1}$  [  $M$  ] and the relative position of  $\mathbf{P}_{j,1}$  with respect to such parent element(s) [  $N_{PE}$  ]

From  $\mathbf{P}_{i,2} = \mathbf{P}_{j,1}$  and along macro-segment  $b$ , proceed to check admissibility of the  $M$  candidates [  $\mathbf{d}_{\xi P} \cdot \bar{\xi}_{k,n}$  ] and select the appropriate reference parent element ( $j$ ) amongst them if necessary, and calculate  $\mathbf{P}_{j,2}$  and  $\mathbf{P}_{j,3}$  via successive linearisations

Repeat sequentially the previous two steps until  $L' \geq L$ , with  $L' = |\mathbf{P}_{q,2} - \mathbf{P}_S|$  and  $L = |\mathbf{P}_E - \mathbf{P}_S|$ , in which case the last embedding parent element has been reached

For each embedded segment  $(\mathbf{P}_S, \mathbf{P}_{i,2}), (\mathbf{P}_{j,1}, \mathbf{P}_{j,2}), \dots, (\mathbf{P}_{q,1}, \mathbf{P}_E)$ , calculate its contribution to stiffness  $\mathbf{K}_{(PE)}^b$  and force vector  $\mathbf{F}_{(PE)}^b$ , with  $PE = i, j, \dots, q$

Figure 4.3: General algorithm structure for the embedment of a macro-segment  $b$

In order to locate the concrete parent element containing  $\mathbf{P}_S$ , a first subset of elements can be filtered from the concrete mesh using a geometric constraint of rapid evaluation. Calling  $\mathbf{C}_{EP}$  the coordinates of the interpolation centroid of a given parent element, and based on a simplification of the sphere defined in Markou and Papadrakakis (2012), the constraint is simply:

$$R_{CN} \geq R_{PS} \quad (4.2)$$

where  $R_{CN}$  represents the maximum distance between the interpolation centroid and an element node, and  $R_{PS}$  is the distance between such centroid and the start point  $\mathbf{P}_S$ . Failing to comply with (4.2) automatically discards the parent element in consideration, whereas satisfaction of (4.2) requires further inspection in order to confirm that  $\mathbf{P}_S$  is contained within (or just on) the parent element boundaries.

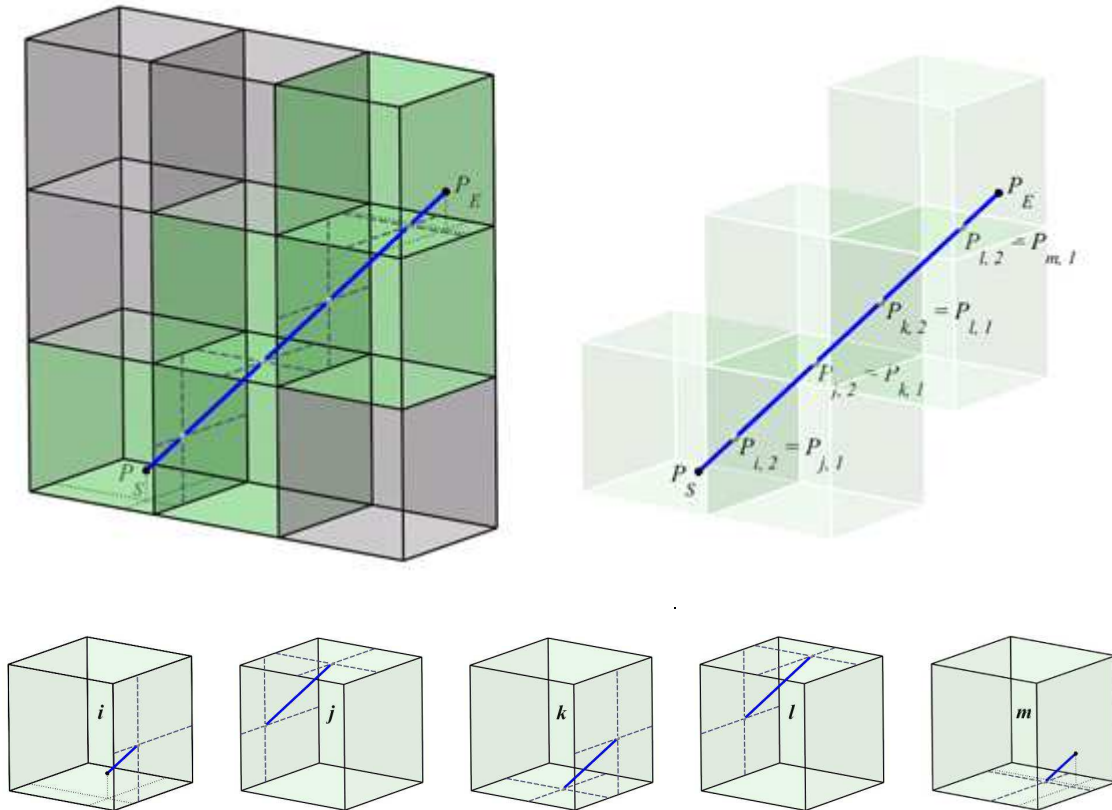


Figure 4.4: (top left) Concrete mesh with bar, highlighting the parent elements actually embedding a segment (top right) Bar and associated embedding elements, marking all points delimiting segments (bottom) Sequence of tracked embedding parent elements

The simplified concrete mesh shown in Figure 4.4 for illustration (whereupon the element nodes have been omitted for clarity, as in the rest of this chapter) comprises exclusively prismatic undistorted elements, and therefore the geometry is maintained between Cartesian  $(X,Y,Z)$  and intrinsic  $(\xi,\eta,\zeta)$  coordinate systems, with the macro-segment traversing prisms as a straight line in both spaces. However, in a more generic approach, the concrete elements display distortions in the Cartesian space, interpolating the geometries allowed by their shape functions. This in turn means that, in the intrinsic coordinate space of a parent element, the embedded segment becomes curved (as shown in Figures 4.5 and 4.6).

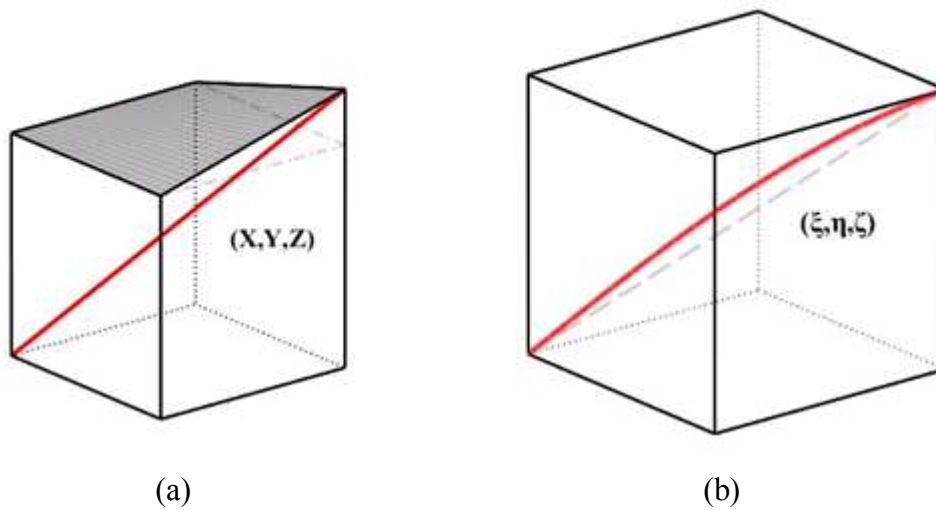


Figure 4.5: (a) 8-noded hexahedron embedding a straight segment, with distortion of the shaded face to become a hyperbolic paraboloid in Cartesian space (b) Normalised element in intrinsic space, embedding a curved segment

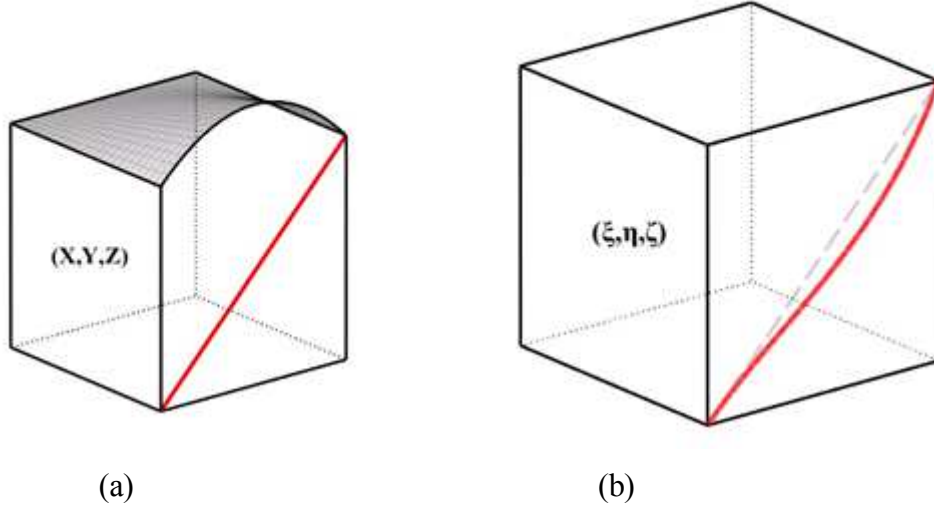


Figure 4.6: (a) 20-noded hexahedron embedding a straight segment, with a parabolic distortion of the shaded face in Cartesian space (b) Normalised element in intrinsic space, embedding a curved segment

Under the general circumstances of a distorted concrete mesh, the relationship between the Cartesian and intrinsic coordinates of an isoparametric parent element, though always explicit in the transformation  $(\xi, \eta, \zeta) \rightarrow (X, Y, Z)$  directly via the shape functions, becomes implicit when transforming  $(X, Y, Z) \rightarrow (\xi, \eta, \zeta)$ . This is of particular relevance when tracking specific points of the embedded segment (in turn potentially expressed at first in terms of its intrinsic one-dimensional coordinate  $r$ ) that require to be expressed in  $(\xi, \eta, \zeta)$  for various purposes, for instance the second level of checking upon satisfaction of (4.2).

Illustratively, a generic point  $\mathbf{P}$ , along the axis of the segment embedded in a prismatic undistorted parent element oriented parallel to the Cartesian axes, can be explicitly determined with intrinsic coordinates:

$$\begin{aligned}\xi_P &= \frac{X_P - X^*}{\frac{\partial X}{\partial \xi}} \\ \eta_P &= \frac{Y_P - Y^*}{\frac{\partial Y}{\partial \eta}} \\ \zeta_P &= \frac{Z_P - Z^*}{\frac{\partial Z}{\partial \zeta}}\end{aligned}\tag{4.3}$$

with  $(X^*, Y^*, Z^*)$  being the Cartesian coordinates of the intrinsic origin ( $\xi = \eta = \zeta = 0$ ). As reference, the intrinsic coordinate systems for all parent element types are shown in Figure 4.7:

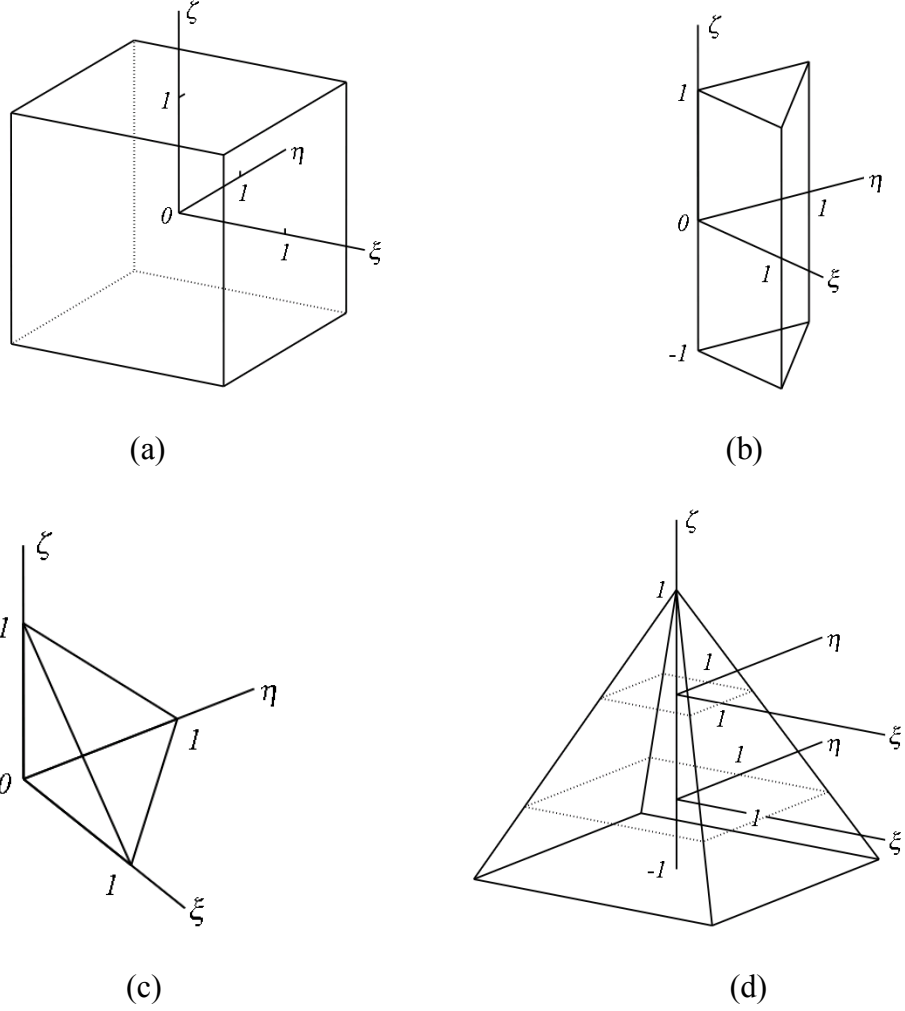


Figure 4.7: Intrinsic coordinate systems for (a) hexahedral (b) wedge (c) tetrahedral (d) pyramidal elements

Rearranged in matrix form, (4.3) becomes:

$$\begin{Bmatrix} \xi \\ \eta \\ \zeta \end{Bmatrix}_P = \begin{bmatrix} \frac{\partial X}{\partial \xi} & 0 & 0 \\ 0 & \frac{\partial Y}{\partial \eta} & 0 \\ 0 & 0 & \frac{\partial Z}{\partial \zeta} \end{bmatrix}^{-1} \cdot \left( \begin{Bmatrix} X \\ Y \\ Z \end{Bmatrix}_P - \begin{Bmatrix} X^* \\ Y^* \\ Z^* \end{Bmatrix} \right) = \bar{\mathbf{J}} \cdot \left( \begin{Bmatrix} X \\ Y \\ Z \end{Bmatrix}_P - \begin{Bmatrix} X^* \\ Y^* \\ Z^* \end{Bmatrix} \right) \quad (4.4)$$

where  $\bar{\mathbf{J}}$  stands for the transposed inverse of the transformation Jacobian. For undistorted elements,  $\bar{\mathbf{J}}$  is constant, thereby allowing the linear explicit relation (4.4). For generically distorted elements, however,  $\bar{\mathbf{J}}$  becomes a function of the unknown intrinsic coordinates  $(\xi, \eta, \zeta)_p$  and hence an iterative procedure becomes necessary to solve the resulting non-linear relation  $(X, Y, Z)_p \rightarrow (\xi, \eta, \zeta)_p$ . Such a procedure, originally derived by Elwi and Hrudey (1989) for two-dimensional elements and later generalised for linear three-dimensional elements by Barzegar and Maddipudi (1994) is called Inverse Mapping and is outlined in the next section. The checking following satisfaction of (4.2) makes use of Inverse Mapping by evaluating if

$$\begin{aligned} & |\xi_{ps}| \leq 1 ; |\eta_{ps}| \leq 1 ; |\zeta_{ps}| \leq 1 \\ & \text{or} \\ & 0 \leq \xi_{ps} \leq 1 ; 0 \leq \eta_{ps} \leq 1 ; |\zeta_{ps}| \leq 1 \\ & \text{or} \\ & 0 \leq \xi_{ps} \leq 1 ; 0 \leq \eta_{ps} \leq 1 ; 0 \leq \zeta_{ps} \leq 1 \end{aligned} \quad (4.5)$$

for every normalised parent element of the filtered subset, whereby the first set of (4.5) applies to hexahedrons and pyramids, the second to wedges and the third to tetrahedrons. Lack of compliance with (4.5) automatically discards the parent element considered. All elements satisfying (4.5) are feasible candidates to embed the first segment: their amount is stored in variable  $M$ , and, for a given candidate, the number of strict equalities arising from (4.5) provides  $N_{PE}$  (Figure 4.3) indicating whether the starting point is embedded, on a face, on an edge or on a vertex node.

### 4.3.2 Inverse Mapping from Cartesian to intrinsic coordinates

The explicit relation  $(\xi, \eta, \zeta)_p \rightarrow (X, Y, Z)_p$  in an isoparametric element is formally expressed in matrix form as:

$$\begin{Bmatrix} X \\ Y \\ Z \end{Bmatrix}_p = \begin{bmatrix} \mathbf{N}(\xi, \eta, \zeta)_p & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{N}(\xi, \eta, \zeta)_p & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{N}(\xi, \eta, \zeta)_p \end{bmatrix} \cdot \begin{Bmatrix} \mathbf{X} \\ \mathbf{Y} \\ \mathbf{Z} \end{Bmatrix} \quad (4.6)$$

where  $\mathbf{N}$  is a vector containing the same shape functions used by the element to interpolate displacements, and  $\{\mathbf{X}, \mathbf{Y}, \mathbf{Z}\}$  are the Cartesian coordinates of the element nodes. By rearranging (4.6) to a homogenous vector equation:

$$\begin{Bmatrix} X \\ Y \\ Z \end{Bmatrix}_P - \begin{Bmatrix} \mathbf{N}(\xi, \eta, \zeta)_P \cdot \mathbf{X} \\ \mathbf{N}(\xi, \eta, \zeta)_P \cdot \mathbf{Y} \\ \mathbf{N}(\xi, \eta, \zeta)_P \cdot \mathbf{Z} \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \end{Bmatrix} \quad (4.7)$$

the sought coordinates  $(\xi, \eta, \zeta)_P$  are the roots of (4.7). If a local standard Newton scheme is applied to this system for iterative resolution, starting from certain initial values  $(\xi, \eta, \zeta)_P^0$ :

$$\begin{Bmatrix} \xi \\ \eta \\ \zeta \end{Bmatrix}_P^0 = \begin{Bmatrix} 0 \\ 0 \\ 0 \end{Bmatrix}_{\text{hexahedron/pyramid}} \quad \text{or} \quad \begin{Bmatrix} \xi \\ \eta \\ \zeta \end{Bmatrix}_P^0 = \begin{Bmatrix} 1/4 \\ 1/4 \\ 0 \end{Bmatrix}_{\text{wedge}} \quad \text{or} \quad \begin{Bmatrix} \xi \\ \eta \\ \zeta \end{Bmatrix}_P^0 = \begin{Bmatrix} 1/4 \\ 1/4 \\ 1/4 \end{Bmatrix}_{\text{tetrahedron}} \quad (4.8)$$

then the  $(i+1)$  iterative correction reads as follows:

$$\begin{Bmatrix} \xi \\ \eta \\ \zeta \end{Bmatrix}_P^{(i+1)} = \begin{Bmatrix} \xi \\ \eta \\ \zeta \end{Bmatrix}_P^{(i)} + \begin{Bmatrix} \Delta\xi \\ \Delta\eta \\ \Delta\zeta \end{Bmatrix}_P^{(i+1)} = \begin{Bmatrix} \xi \\ \eta \\ \zeta \end{Bmatrix}_P^{(i)} + \bar{\mathbf{J}}^{(i)} \cdot \left( \begin{Bmatrix} X \\ Y \\ Z \end{Bmatrix}_P - \begin{Bmatrix} \mathbf{N}^{(i)} \cdot \mathbf{X} \\ \mathbf{N}^{(i)} \cdot \mathbf{Y} \\ \mathbf{N}^{(i)} \cdot \mathbf{Z} \end{Bmatrix} \right) \quad (4.9)$$

with  $\mathbf{N}^{(i)} = \mathbf{N}(\xi, \eta, \zeta)_P^{(i)}$  and:

$$\bar{\mathbf{J}}^{(i)} = \begin{bmatrix} \frac{\partial X}{\partial \xi} & \frac{\partial X}{\partial \eta} & \frac{\partial X}{\partial \zeta} \\ \frac{\partial Y}{\partial \xi} & \frac{\partial Y}{\partial \eta} & \frac{\partial Y}{\partial \zeta} \\ \frac{\partial Z}{\partial \xi} & \frac{\partial Z}{\partial \eta} & \frac{\partial Z}{\partial \zeta} \end{bmatrix}^{-1, (i)} = \left( \sum_{n=1}^{ne} \begin{bmatrix} \frac{\partial \mathbf{N}_n^{(i)}}{\partial \xi} \mathbf{X}_n & \frac{\partial \mathbf{N}_n^{(i)}}{\partial \eta} \mathbf{X}_n & \frac{\partial \mathbf{N}_n^{(i)}}{\partial \zeta} \mathbf{X}_n \\ \frac{\partial \mathbf{N}_n^{(i)}}{\partial \xi} \mathbf{Y}_n & \frac{\partial \mathbf{N}_n^{(i)}}{\partial \eta} \mathbf{Y}_n & \frac{\partial \mathbf{N}_n^{(i)}}{\partial \zeta} \mathbf{Y}_n \\ \frac{\partial \mathbf{N}_n^{(i)}}{\partial \xi} \mathbf{Z}_n & \frac{\partial \mathbf{N}_n^{(i)}}{\partial \eta} \mathbf{Z}_n & \frac{\partial \mathbf{N}_n^{(i)}}{\partial \zeta} \mathbf{Z}_n \end{bmatrix} \right)^{-1} \quad (4.10)$$

$$\bar{\mathbf{J}}^{(i)} = \left( \sum_{n=1}^{ne} \begin{Bmatrix} \mathbf{X}_n \\ \mathbf{Y}_n \\ \mathbf{Z}_n \end{Bmatrix} \otimes \begin{bmatrix} \frac{\partial \mathbf{N}_n^{(i)}}{\partial \xi} & \frac{\partial \mathbf{N}_n^{(i)}}{\partial \eta} & \frac{\partial \mathbf{N}_n^{(i)}}{\partial \zeta} \end{bmatrix} \right)^{-1}$$

with  $ne$  signifying the number of nodes in a given element. Iterations continue until the residual falls below a certain predefined threshold, at which point the triplet as corrected by the last iteration cycle is accepted as  $(\xi, \eta, \zeta)_P$ . Barzegar and Maddipudi (1994) reported a high convergence rate for linear hexahedrons, and this has been corroborated here for all four types of quadratic element, whereby convergence is ensured provided distortions are not unreasonable (Hartl, 2002).

### 4.3.3 Sequential tracking of intersection points for macro-segment discretisation

Once a group of feasible candidates or a single reference parent element thereof has been selected as the one embedding  $\mathbf{P}_S$ , as elaborated in Section 4.3.3.1, it is necessary to track along the bar axis all its successive intersection points with the traversed parent element faces. This serves the purpose of discretising the macro-segment in a consistent manner with the concrete mesh. In general, a certain parent element  $k$  has two intersection points, i.e. an *entry* ( $\mathbf{P}_{k,1}$ ) and an *exit* ( $\mathbf{P}_{k,2}$ ) point, considering the *forward* direction as the one given by  $\mathbf{d}_{SE}$ . The only exceptions to this are the extreme elements embedding  $\mathbf{P}_S$  or  $\mathbf{P}_E$  (or potentially both). Consequently, for any pair of adjacent parent elements  $\{k, l\}$ , embedding consecutive segments of a given bar the following is of general validity:

$$\mathbf{P}_{k,2} = \mathbf{P}_{l,1} \quad (4.11)$$

as can be seen from Figure 4.4.

In order to sequentially find point  $\mathbf{P}_{k,2}$  given that  $\mathbf{P}_{k,1}$  is known for any generic parent element  $k$ , a tracking procedure is proposed. It is notionally based on the approach of Barzegar and Maddipudi (1994), and later Huber (2006), who dealt exclusively with linear hexahedrons. However, their tracking method is formulated in Cartesian space and considers the parent element faces to be always represented by planes, the intersection of which with the macro-segment provides the sought points. As shown in Figure 4.5a, even linear 8-noded hexahedrons can accommodate distorted (non-planar) face geometries in the shape of a hyperbolic paraboloid, and hence the method can potentially introduce an approximation and is not necessarily exact, as deemed by these authors. With quadratic elements, this issue can only be accentuated. Furthermore, Huber (2006) introduced an additional approximation by simplifying the embedded segment in intrinsic coordinate space, substituting the spatial curve by its chord (Figure 4.5b).

As Hartl (2002) resorted to quadratic hexahedrons, the aforementioned issues were addressed by shifting the tracking coordinate space from Cartesian to intrinsic, and this is the approach followed and enhanced hereafter.

#### 4.3.3.1 Selection of admissible parent elements

Establishing the framework of the tracking procedure in the intrinsic coordinate space has the immediate advantage that all normalised parent element faces become planes, with well-defined and constant outer normals  $\bar{\xi}_{j,n}$ , where  $j$  ranges between 1 and the number of faces, depending on the element type. For hexahedral elements, all faces are expressed as  $\xi/\eta/\zeta = \pm 1$  (Figure 4.8) and the corresponding outer normals are:

$$\bar{\xi}_{1,n}^{hex} = -\bar{\xi}_{4,n}^{hex} = \begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix}; \bar{\xi}_{2,n}^{hex} = -\bar{\xi}_{5,n}^{hex} = \begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix}; \bar{\xi}_{3,n}^{hex} = -\bar{\xi}_{6,n}^{hex} = \begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix} \quad (4.12)$$

As reference, all remaining element types and outer normals are schematically represented in Figures 4.9 to 4.11 and (4.13) to (4.15).

$$\bar{\xi}_{1,n}^{tet} = \begin{Bmatrix} 0 \\ -1 \\ 0 \end{Bmatrix}; \bar{\xi}_{2,n}^{tet} = \begin{Bmatrix} -1 \\ 0 \\ 0 \end{Bmatrix}; \bar{\xi}_{3,n}^{tet} = \begin{Bmatrix} 0 \\ 0 \\ -1 \end{Bmatrix}; \bar{\xi}_{4,n}^{tet} = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix} \quad (4.13)$$

$$\bar{\xi}_{1,n}^{wed} = \begin{Bmatrix} 0 \\ -1 \\ 0 \end{Bmatrix}; \bar{\xi}_{2,n}^{wed} = \begin{Bmatrix} -1 \\ 0 \\ 0 \end{Bmatrix}; \bar{\xi}_{3,n}^{wed} = \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix}; \bar{\xi}_{4,n}^{wed} = \begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix}; \bar{\xi}_{5,n}^{wed} = \begin{Bmatrix} 0 \\ 0 \\ -1 \end{Bmatrix} \quad (4.14)$$

$$\bar{\xi}_{1,n}^{pyr} = \begin{Bmatrix} 0 \\ 0 \\ -1 \end{Bmatrix}; \bar{\xi}_{2,n}^{pyr} = \begin{Bmatrix} 2 \\ 0 \\ 1 \end{Bmatrix}; \bar{\xi}_{3,n}^{pyr} = \begin{Bmatrix} 0 \\ -2 \\ 1 \end{Bmatrix}; \bar{\xi}_{4,n}^{pyr} = \begin{Bmatrix} -2 \\ 0 \\ 1 \end{Bmatrix}; \bar{\xi}_{5,n}^{pyr} = \begin{Bmatrix} 0 \\ 2 \\ 1 \end{Bmatrix} \quad (4.15)$$

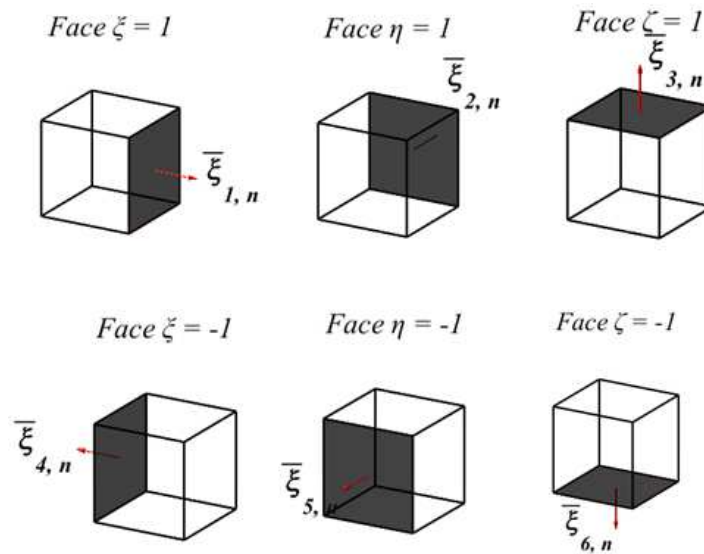


Figure 4.8: Faces and outer normals of a normalised hexahedron

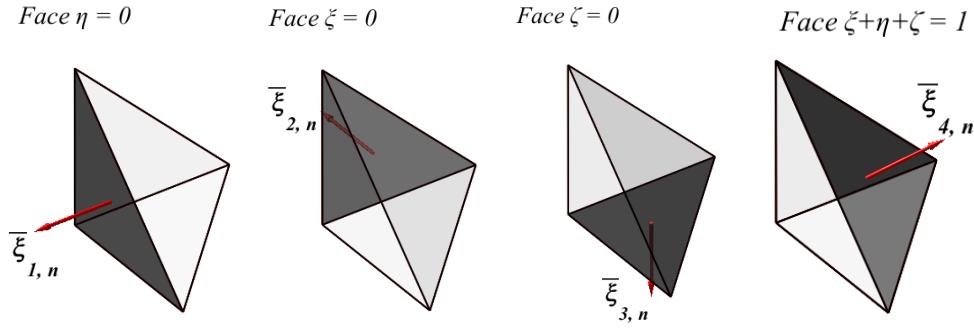


Figure 4.9: Faces and outer normals of a normalised tetrahedron

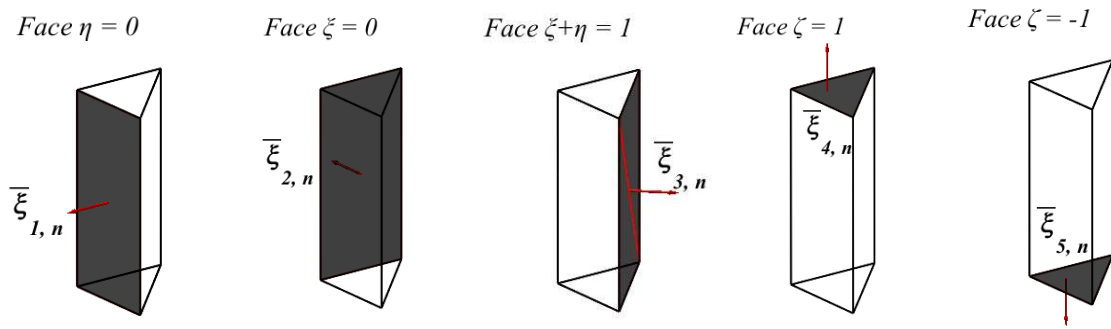


Figure 4.10: Faces and outer normals of a normalised wedge

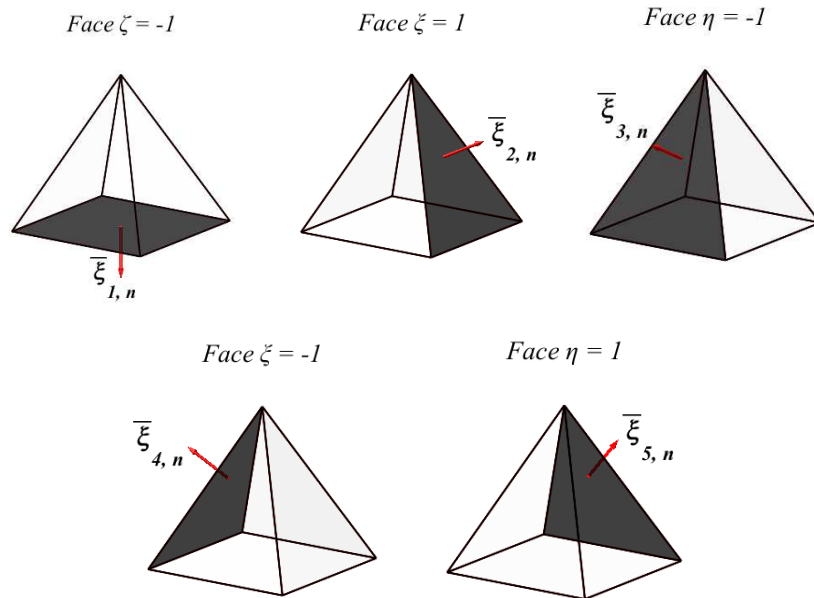


Figure 4.11: Faces and outer normals of a normalised pyramid

In Section 4.3.1, it was shown that in general the embedded segment loses its straight geometry in the intrinsic coordinate space and becomes a spatial curve instead. Thus, whilst working in such a space renders constant outer normals  $\bar{\xi}_{j,n}$ , the axial segment direction  $\mathbf{d}_{\hat{\xi},P}$  becomes a function of the point  $P$  considered along the bar:

$$\mathbf{d}_{\hat{\xi},P} = \bar{\mathbf{J}}(\zeta, \eta, \zeta)_P \cdot \mathbf{d}_{SE} \quad (4.16)$$

The invariant dot product  $(\mathbf{d}_{\hat{\xi},P} \cdot \bar{\xi}_{j,n})$ , however, proves more advantageous in this space rather than the Cartesian one as it provides a final tool to discern the reference admissible element from the subset of feasible candidates sharing  $\mathbf{P}_S$  (or, more generically for subsequent parent elements,  $\mathbf{P}_{k,1}$ ) in a straightforward manner, simply by checking:

$$\begin{aligned} \mathbf{d}_{\hat{\xi},P_S} \cdot \bar{\xi}_{j,n} &= (\bar{\mathbf{J}}(\zeta, \eta, \zeta)_{P_S} \cdot \mathbf{d}_{SE}) \cdot \bar{\xi}_{j,n} \leq 0 \\ \text{or, for subsequent parent elements:} \\ \mathbf{d}_{\hat{\xi},P_{k,l}} \cdot \bar{\xi}_{j,n} &= (\bar{\mathbf{J}}(\zeta, \eta, \zeta)_{P_{k,l}} \cdot \mathbf{d}_{SE}) \cdot \bar{\xi}_{j,n} \leq 0 \end{aligned} \quad (4.17)$$

This is shown illustratively in Figure 4.12, where the same regular undistorted concrete mesh as in Figure 4.4 embeds a macro-segment that intersects parent elements at the edges. Once parent element  $i$  is identified as the one embedding  $\mathbf{P}_S$  and exit point  $\mathbf{P}_{i,2}$  is tracked, there is a subset of 3 adjacent feasible candidates  $\{j, k, n\}$  (as per adjacency considerations discussed in Section 4.3.3.3) to embed the subsequent segment, as all of them satisfy (4.5) after Inverse Mapping. Figure 4.13 depicts this subset, along with the vectors of each candidate entering the dot product checks (4.17).

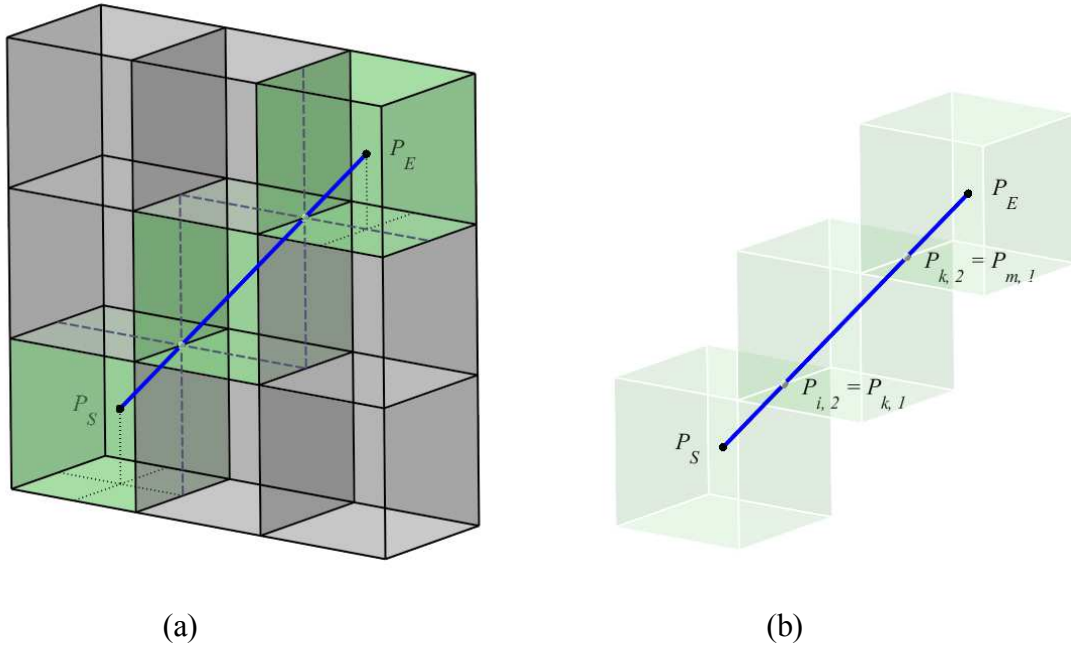


Figure 4.12: (a) Concrete mesh with bar, highlighting the parent elements actually embedding a segment (b) Bar and associated embedding elements, marking all points delimiting segments

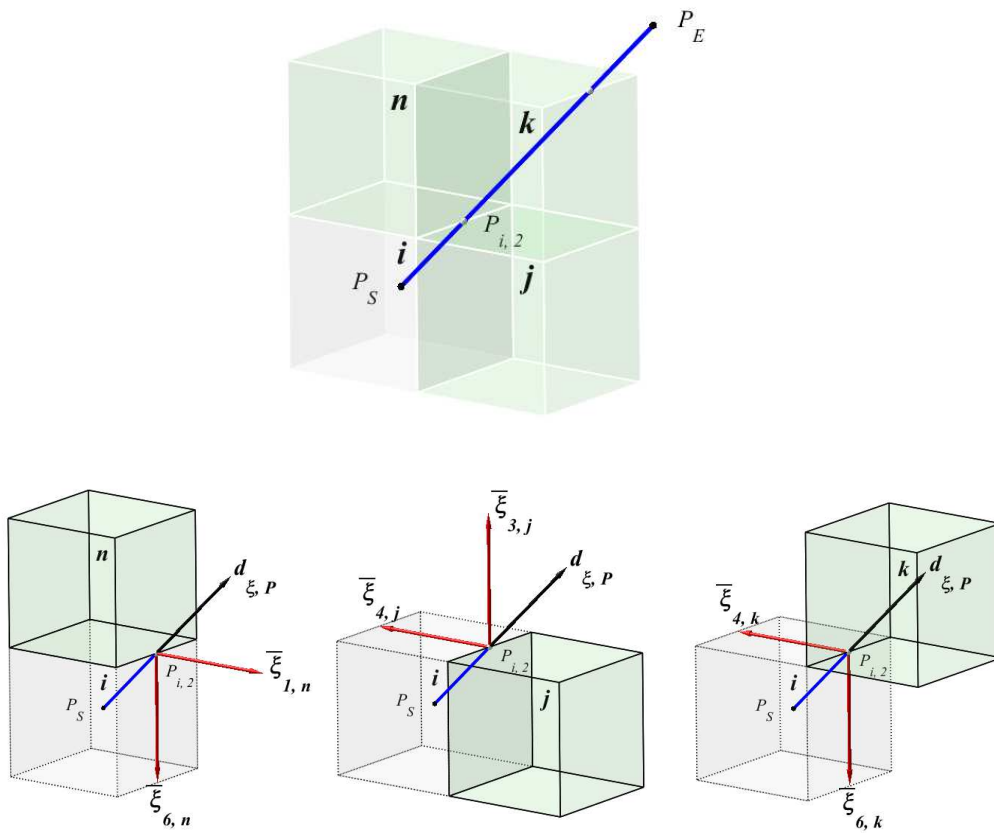


Figure 4.13: (top) Subset of feasible candidates to embed the segment starting at  $P_{i,2}$  (bottom) Evaluation of dot products to assess admissibility of candidates

As the concrete mesh is prismatic and undistorted, the Cartesian and intrinsic coordinate spaces are homothetic in this case, although strictly speaking (4.17) is performed in the latter. Since a positive dot product automatically implies that a candidate should be deemed inadmissible, (4.17) leads directly to parent element  $k$  as the reference one embedding the next bar segment in Figure 4.13. It is worth noting that this is achieved in this work without changing conditions (4.5) and then calculating a further intersection, as originally proposed in Hartl (2002). For each candidate, the number of dot products contained in (4.17) coincides with  $N_{PE}$  (Figure 4.3), i.e. the number of strict equalities arising from (4.5).

A further advantage of the proposed formulation in (4.17) is that distinguishing between dot products satisfying the check as equality or inequality allows to formally classify all potential cases in a systematic manner, which can be extended to all parent element types. This is enabled by the fact that any element edge connects 2 of its faces and, analogously, any element vertex node connects 3 of its faces. The apex of a pyramid element constitutes the only exception to this, and is discussed separately in Section 4.3.4. Table 4.1 shows all formal cases of a segment entering a parent element through  $\mathbf{P}_{i,1}$  as a function of  $N_{PE}$  and the dot products (4.17).

| $N_{PE}$ | Dot product(s)                                                                                                                                                       | Case | Description                                                                                |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|--------------------------------------------------------------------------------------------|
| 0        | —                                                                                                                                                                    | 0    | First segment of the bar, 'entry' point $\mathbf{P}_s$ is <i>inside</i> the parent element |
| 1        | $\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{j,n} < 0$                                                                                                                 | I    | Segment enters through a FACE into the bulk of the parent element                          |
| 2        | $\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{j,n} < 0$<br>$\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{k,n} < 0$                                                         | II   | Segment enters through an EDGE into the bulk of the parent element                         |
| 3        | $\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{j,n} < 0$<br>$\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{k,n} < 0$<br>$\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{l,n} < 0$ | III  | Segment enters through a NODE into the bulk of the parent element                          |
| 2        | $\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{j,n} < 0$<br>$\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{k,n} = 0$                                                         | IV   | Segment enters through an EDGE tangentially to a FACE                                      |
| 3        | $\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{j,n} < 0$<br>$\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{k,n} < 0$<br>$\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{l,n} = 0$ | V    | Segment enters through a NODE tangentially to a FACE                                       |
| 3        | $\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{j,n} < 0$<br>$\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{k,n} = 0$<br>$\mathbf{d}_{\xi, P_{i1}} \cdot \bar{\xi}_{l,n} = 0$ | VI   | Segment enters through a NODE tangentially to an EDGE                                      |

Table 4.1: Formal cases of segment entering a parent element

Whilst for cases II-III the dot product checks (4.17) suffice to establish the reference parent element embedding the entering segment (case I is trivial as the set of feasible candidates consists of only one element from the start), cases IV-VI involve more than one admissible parent element. Hence, an additional check of the relevant condition (4.5) applied to the tracked exit point is required *a posteriori* to establish which of the admissible elements is the reference one, i.e. admissible elements are consecutively checked via:

$$\begin{aligned}
 & |\xi_{Pi,2}| \leq 1 ; |\eta_{Pi,2}| \leq 1 ; |\zeta_{Pi,2}| \leq 1 \\
 & \text{or} \\
 & 0 \leq \xi_{Pi,2} \leq 1 ; 0 \leq \eta_{Pi,2} \leq 1 ; |\zeta_{Pi,2}| \leq 1 \\
 & \text{or} \\
 & 0 \leq \xi_{Pi,2} \leq 1 ; 0 \leq \eta_{Pi,2} \leq 1 ; 0 \leq \zeta_{Pi,2} \leq 1
 \end{aligned} \tag{4.18}$$

The procedure can even accommodate the special circumstance of more than one admissible element satisfying (4.18), which geometrically means that an entire segment is embedded along a shared element face or a shared element edge (Figure 4.14). In such case, the segment is solely assigned to the first parent element satisfying (4.18), for the purpose of calculating its contribution to the parent element stiffness and force vector (elaborated in Section 4.4). This has been considered sufficient in the present work, although it is also possible to distribute these contributions amongst the admissible elements sharing the segment, as in Markou and Papadrakakis (2012). This approach, however, is unnecessary as far the resistance of the embedded segment is concerned.

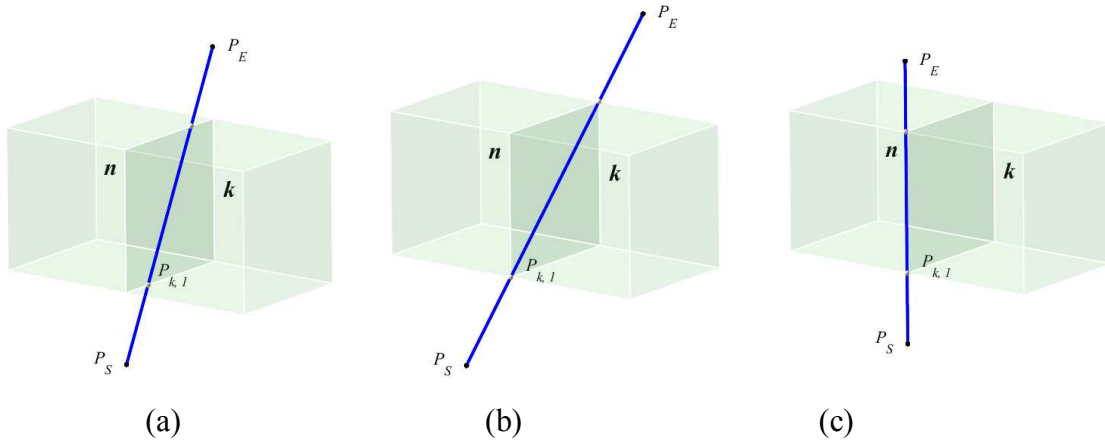


Figure 4.14: Segment evolving along a shared face: (a) Case IV (b) Case V. Segment evolving along a shared edge: (c) Case VI. In all cases the segment is assumed to be embedded solely in element  $k$ , as the first one to satisfy (4.18)

### 4.3.3.2 Sequential linearisations

Following the usual approach when facing the resolution of a nonlinear problem, the tracing of intersection (exit) point  $\mathbf{P}_{k,2}$  in a generic parent element  $k$  starting from a known (entry) point  $\mathbf{P}_{k,1}$  resorts to the sequence of linearisations characteristic of a standard Newton scheme. As introduced in the previous section, this process takes place in the intrinsic coordinate space of the parent element, where a first linearisation from  $\mathbf{P}_{k,1}$ , recalling (4.16) and (4.1), leads to the following increment of intrinsic coordinates:

$$\begin{Bmatrix} \Delta\zeta \\ \Delta\eta \\ \Delta\zeta \end{Bmatrix} = \bar{\mathbf{J}}(\zeta, \eta, \zeta)_{P_{k,1}} \cdot \begin{Bmatrix} \Delta X \\ \Delta Y \\ \Delta Z \end{Bmatrix} = \bar{\mathbf{J}}(\zeta, \eta, \zeta)_{P_{k,1}} \cdot \Delta\alpha \begin{Bmatrix} l_1 \\ m_1 \\ n_1 \end{Bmatrix} \quad (4.19)$$

where  $\Delta\alpha$  is the length of the linearised prediction of the segment in Cartesian space. Depending on the element type and the case (Table 4.1), different faces (in spatial definition and number) are considered for the tracking of their intersection with the linearised segment as per (4.19). Table 4.2 summarises all possible options in this regard.

If the relevant element face is expressed as:

$$\hat{\xi}_i = c, \quad c = \begin{cases} 1 \\ 0 \\ -1 \end{cases} \quad (4.20)$$

with  $\hat{\xi} = \{\zeta, \eta, \zeta\}^t$ , then one intrinsic coordinate increment in (4.19) can be expressed as:

$$\Delta\hat{\xi}_i = c - (\hat{\xi}_i)_{k,1} \quad (4.21)$$

The remaining increments arise from solving system (4.19), determinate once an element face has been chosen. In particular, the resultant length of the linearised segment reads:

$$\Delta\alpha = \frac{\Delta\hat{\xi}_i}{\bar{\mathbf{J}}_{i1} \cdot l_1 + \bar{\mathbf{J}}_{i2} \cdot m_1 + \bar{\mathbf{J}}_{i3} \cdot n_1} \quad (4.22)$$

Most element faces in intrinsic coordinate space comply with definition (4.20). However, in wedge and tetrahedral elements, there are faces not perpendicular to the coordinate axes, expressed as:

$$\zeta + \eta = \hat{\xi}_1 + \hat{\xi}_2 = 1 \quad (4.23)$$

| Case | Number of faces $N_f$ considered |         |             |         | Description                                                                                                       |
|------|----------------------------------|---------|-------------|---------|-------------------------------------------------------------------------------------------------------------------|
|      | Hexahedron                       | Wedge   | Tetrahedron | Pyramid |                                                                                                                   |
| 0    | 6                                | 5       | 4           | 5       | All element faces are considered                                                                                  |
| I    | 5                                | 4       | 3           | 4       | The 1 entry face is not considered                                                                                |
| II   | 4                                | 3       | 2           | 3       | The 2 faces sharing the entry edge are not considered                                                             |
| III  | 3                                | 2       | 1           | 2(*)    | The 3 faces sharing the entry node are not considered                                                             |
| IV   | 3                                | 2/3(**) | 2           | 2/3(**) | Consider only the $N_f$ faces surrounding the shared face and not containing the entry edge                       |
| V    | 2                                | 1/2(**) | 1           | 1/2(**) | Consider only the $N_f$ faces surrounding the shared face and not containing the entry node                       |
| VI   | 1                                | 1       | 1           | 1(***)  | Consider only 1 face, opposite the entry node in the direction of the edge tangentially approached by the segment |

Table 4.2: Number of parent element faces checked for intersection with the first linearisation of the segment, as a function of the element type and the applicable case (\*) Nodes not being the apex (\*\*) Number depends on the shared face being triangular (left) or quadrilateral (right) (\*\*\*) If the tangential direction is not that of one of the square base edges, the intersection is assumed to be at the apex

and:

$$\zeta + \eta + \zeta = \hat{\xi}_1 + \hat{\xi}_2 + \hat{\xi}_3 = 1 \quad (4.24)$$

respectively. Analogous operations as in (4.21) and (4.22) lead in turn to:

$$\Delta\alpha = \frac{1 - \left(\hat{\xi}_1\right)_{k,1} - \left(\hat{\xi}_2\right)_{k,1}}{\left(\bar{\mathbf{J}}_{11} + \bar{\mathbf{J}}_{21}\right) \cdot l_1 + \left(\bar{\mathbf{J}}_{12} + \bar{\mathbf{J}}_{22}\right) \cdot m_1 + \left(\bar{\mathbf{J}}_{13} + \bar{\mathbf{J}}_{23}\right) \cdot n_1} \quad (4.25)$$

$$\Delta\alpha = \frac{1 - \left(\hat{\xi}_1\right)_{k,1} - \left(\hat{\xi}_2\right)_{k,1} - \left(\hat{\xi}_3\right)_{k,1}}{\left(\bar{\mathbf{J}}_{11} + \bar{\mathbf{J}}_{21} + \bar{\mathbf{J}}_{31}\right) \cdot l_1 + \left(\bar{\mathbf{J}}_{12} + \bar{\mathbf{J}}_{22} + \bar{\mathbf{J}}_{32}\right) \cdot m_1 + \left(\bar{\mathbf{J}}_{13} + \bar{\mathbf{J}}_{23} + \bar{\mathbf{J}}_{33}\right) \cdot n_1} \quad (4.26)$$

Once all  $N_f$  element faces have been considered as per Table 4.2, if  $N_f > 1$  the appropriate value of  $\Delta\alpha$  must be selected, corresponding to the closest intersection in the *forward* direction (i.e. the minimum  $\Delta\alpha$ ). Since this intersection point represents the *exit* point of the linearised segment, checking for the minimum  $\Delta\alpha$  is equivalent to checking which intersection point satisfies (4.18). This minimum, however, is selected amongst the positive values of  $\Delta\alpha$ , as a negative value indicates that the linearised segment intersects a face only in the *backward* direction.

Figures 4.15 and 4.16 illustrate this for a segment embedded in a distorted hexahedral parent element  $k$  under formal case I (Table 4.2). Although the number of accounted element faces is  $N_f = 5$ , only 3 intersections are shown in Figure 4.16 for clarity, as the remaining 2 element faces are parallel to the plane containing the linearised segment and hence  $\Delta\alpha \rightarrow \infty$ .

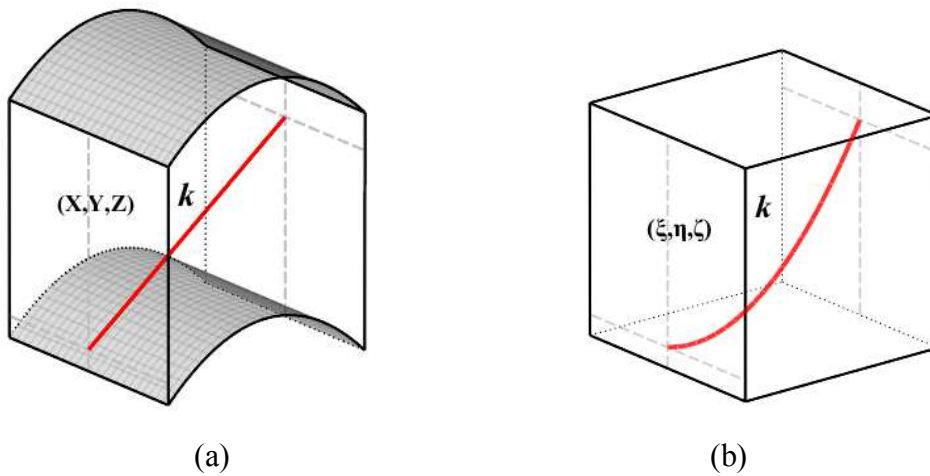


Figure 4.15: Embedded segment and hexahedral parent element  $k$  in (a) Cartesian space  
(b) intrinsic coordinate space

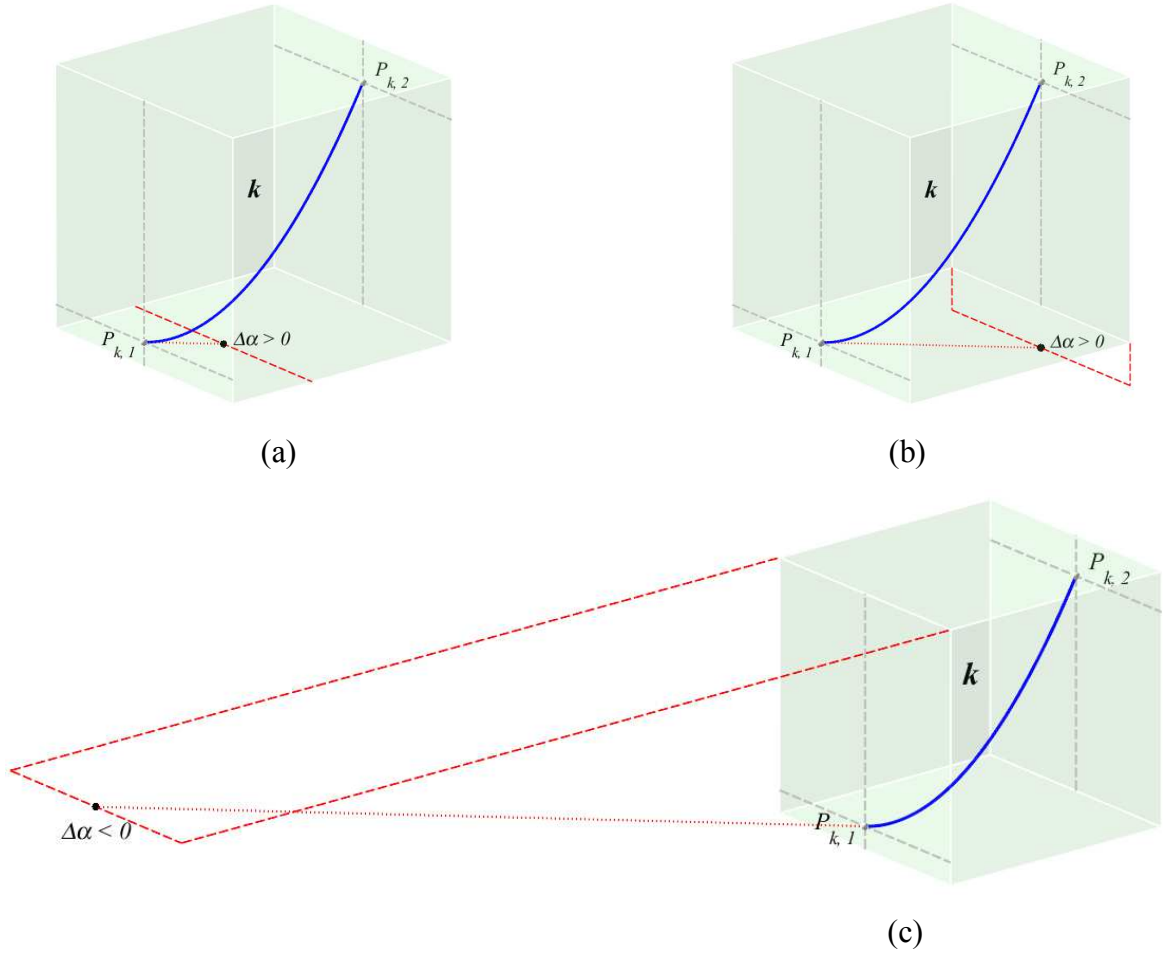


Figure 4.16: Intersections of the first segment linearisation with the faces of parent element  $k$  in intrinsic coordinate space (a) Admissible with  $\Delta\alpha = \Delta\alpha_{\min}$  (b) Admissible with  $\Delta\alpha > \Delta\alpha_{\min}$  (c) Inadmissible with  $\Delta\alpha < 0$

Substitution of  $\Delta\alpha = \Delta\alpha_{\min}$  in equation (4.19) leads to the closest admissible intersection point  $P_{k,L1}^{PE}$  of the linearised segment with a parent element face:

$$\mathbf{P}_{k,L1}^{PE} = \left( \hat{\xi} \right)_{k,1} + \Delta \hat{\xi}_{L1} \quad (4.27)$$

initially in intrinsic coordinates although an isoparametric transformation via (4.6) readily provides the equivalent Cartesian coordinates. On the other hand, from the perspective of the segment,  $\Delta\alpha = \Delta\alpha_{\min}$  leads to the point  $P_{k,L1}^b$  along the axis of the bar:

$$\mathbf{P}_{k,L1}^b = \mathbf{P}_{k,1} + \Delta\alpha_{\min} \mathbf{d}_{SE} \quad (4.28)$$

directly in Cartesian coordinates. In general, points (4.27) and (4.28) do not coincide. Only in the case of prismatic undistorted parent elements does a single linearization suffice as

$\mathbf{P}_{k,L1}^{PE} \equiv \mathbf{P}_{k,L1}^b = \mathbf{P}_{k,2}$  due to the constant  $\bar{\mathbf{J}}$  in the whole element domain, whereby  $\mathbf{P}_{k,L1}^{PE}$  needs to be transformed to Cartesian coordinates. For any other case,  $\mathbf{P}_{k,L1}^b$  is taken as the new reference point (upon transformation to intrinsic coordinates) from where to continue linearising, giving rise each time to a new pair of points  $(\mathbf{P}_{k,Lj}^{PE}, \mathbf{P}_{k,Lj}^b)$ . Tracking the distance between them, which formally plays the role of a residual, convergence is considered to be achieved upon their spatial coincidence (within a prescribed tolerance). This is illustratively shown in Figure 4.17 for the same case depicted in Figure 4.15, where the third linearisation already renders  $\mathbf{P}_{k,L3}^{PE} \equiv \mathbf{P}_{k,L3}^b = \mathbf{P}_{k,2}$  within tolerance.

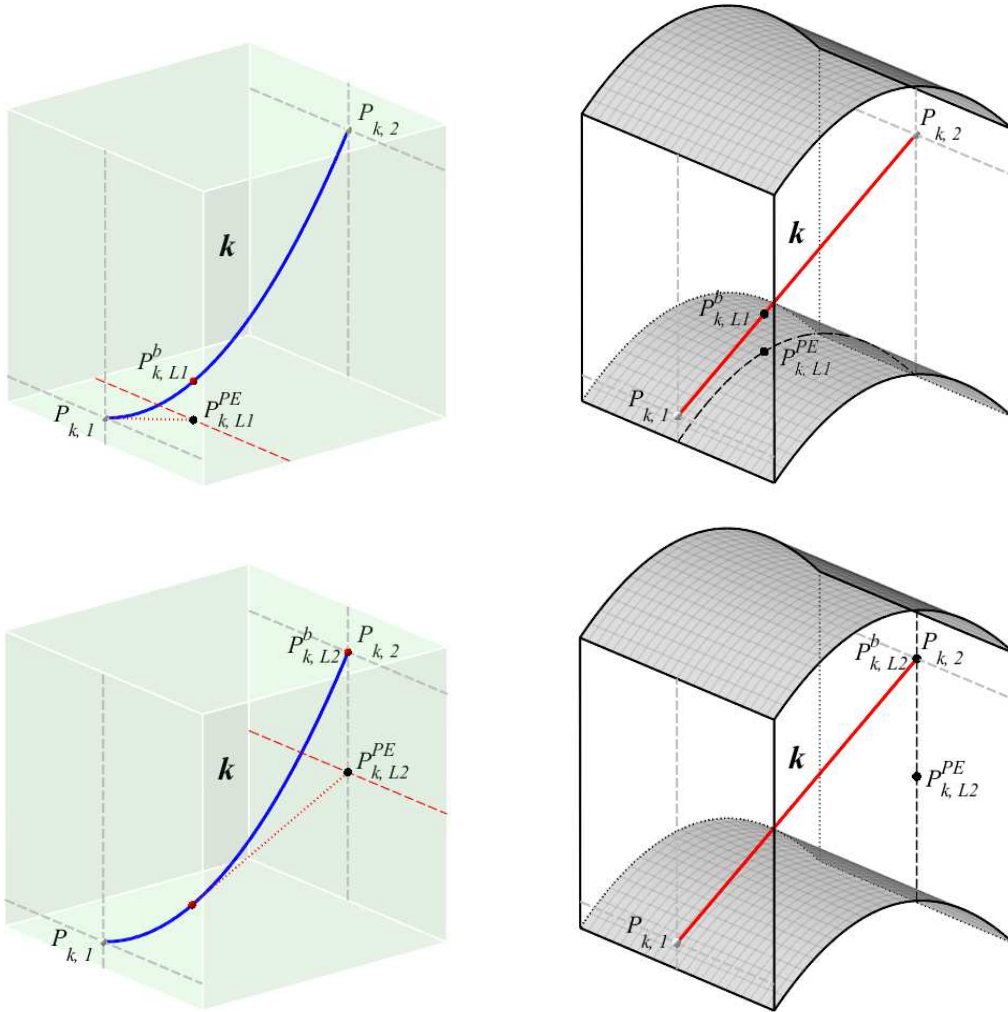


Figure 4.17: Evolution of two linearisations in parent element  $k$  intrinsic coordinate space (left) and Cartesian space (right)

The only formal differences between linearisations  $L1$  and any subsequent  $Lj$  are that, in the latter, Case 0 (Table 4.2) is restored for any parent element type (i.e. in the example,  $N_f = 6$

for  $j > 1$ ) as, from a certain level of distortion on, it is feasible that a segment exits the parent element through the same face containing the entry point  $\mathbf{P}_{k,1}$ . Also, under the same considerations of distortion, point  $\mathbf{P}_{k,Lj}^b$  with  $j > 1$  can potentially lie outside of the parent element boundaries (by not satisfying relevant conditions (4.18) applied to this point). In that circumstance, linearisation  $(j+1)$  must invert the admissibility criterion for  $\Delta\alpha$ , taking only into account negative values from which the maximum is selected.

Hence, for a generic subsequent linearisation  $(j > 1)$ , the relevant pair of points is obtained as:

$$\mathbf{P}_{k,Lj}^{PE} = \left( \hat{\xi} \right)_{k,L(j-1)}^b + \Delta \hat{\xi}_{Lj} \quad (4.29)$$

$$\mathbf{P}_{k,Lj}^b = \mathbf{P}_{k,L(j-1)}^b + \Delta\alpha_{\min} \mathbf{d}_{SE} \quad (4.30)$$

with:

$$\Delta\alpha_{\min} = \min \left( |\Delta\alpha_1|, \dots, |\Delta\alpha_{N_f}| \right) \quad (4.31)$$

and:

$$\text{admissible } \Delta\alpha = \begin{cases} > 0 & \text{if } \mathbf{P}_{k,L(j-1)}^b \in PE(k) \\ < 0 & \text{if } \mathbf{P}_{k,L(j-1)}^b \notin PE(k) \end{cases} \quad (4.32)$$

whereby the process is repeated until  $\mathbf{P}_{k,Lj}^{PE} \simeq \mathbf{P}_{k,Lj}^b$  within a prescribed tolerance, and such coordinates are assigned to  $\mathbf{P}_{k,2}$ . Recalling (4.11), this also constitutes the entry point to the next parent element, embedding the continuing bar segment.

#### 4.3.3.3 Adjacency criteria for continuation of the tracking procedure

Once exit point  $\mathbf{P}_{k,2}$  has been established within parent element  $k$ , a feasible set of parent element candidates to embed the subsequent segment is produced based on adjacency considerations. To this end,  $N_{PE}$  (Figure 4.3) evaluated at the exit point (as the number of strict equalities in (4.18)) provides the number of adjacency corner nodes  $(4 - N_{PE})$  necessary to establish which parent elements form the set. As an example, Figure 4.18 shows a partition of a regular hexahedral mesh with all possibilities of  $N_{PE}$  at  $\mathbf{P}_{k,2}$ .

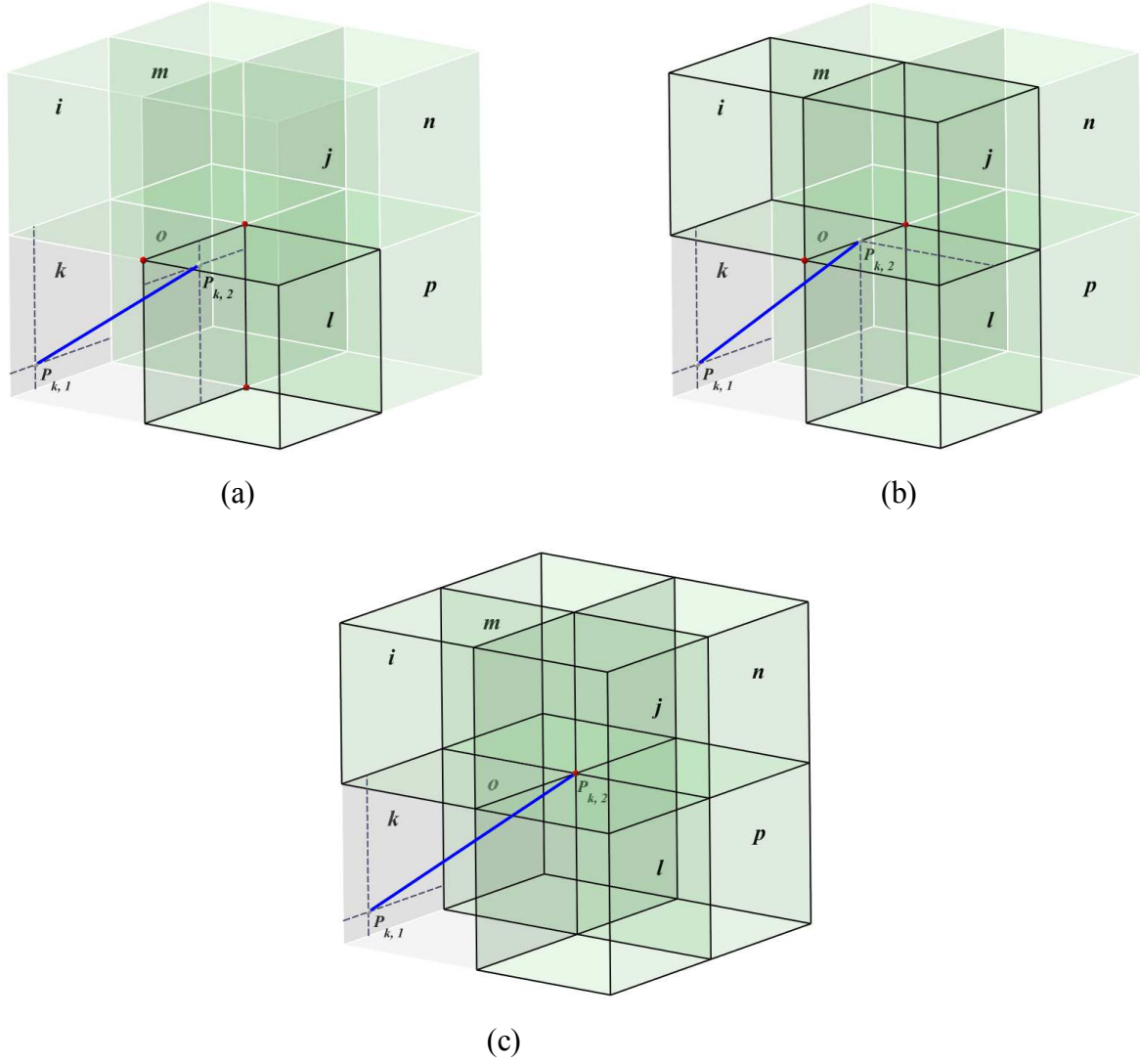


Figure 4.18: Subset of a hexahedral concrete mesh in Cartesian space, with a segment exiting parent element  $k$  with (a)  $N_{PE}=1$  (b)  $N_{PE}=2$  (c)  $N_{PE}=3$ . Adjacency nodes marked in red and feasible candidates to embed the next segment highlighted in black

Only when  $N_{PE}=1$  can the subsequent parent element be determined uniquely, as there can be only one adjacent element sharing at least 3 corner nodes with parent element  $k$ . For all other cases, depending on the element type and mesh geometry, a certain number of candidates  $M$  share the 2 corner nodes of a common edge or the one common corner node. In order to find out which parent element is admissible amongst the  $M$  candidates, checking of dot products (4.17) is required.

#### 4.3.3.4 End of the tracking procedure

The described procedure to find the exit point  $\mathbf{P}_{k,2}$  for any parent element  $k$  traversed by a given macro-segment  $b$  is ended when the parent element embedding  $\mathbf{P}_E$  is reached. To check this, every time a parent element (including the very first one, embedding  $\mathbf{P}_S$ ) is evaluated for an exit point the distance  $L'$  in Cartesian space between that point and  $\mathbf{P}_S$  is compared with the given macro-segment length  $L$ . Alternatively,  $L'$  can be regarded as the cumulative sum of all  $\Delta\alpha_{\min}$  obtained for  $b$  up to the stage in consideration. Whenever  $L' \geq L$  is satisfied, the procedure is ended for macro-segment  $b$ , with  $\mathbf{P}_E$  substituting the last computed exit point. Figure 4.19 shows a basic example of this, where all parent elements other than the extreme ones have been omitted for clarity.

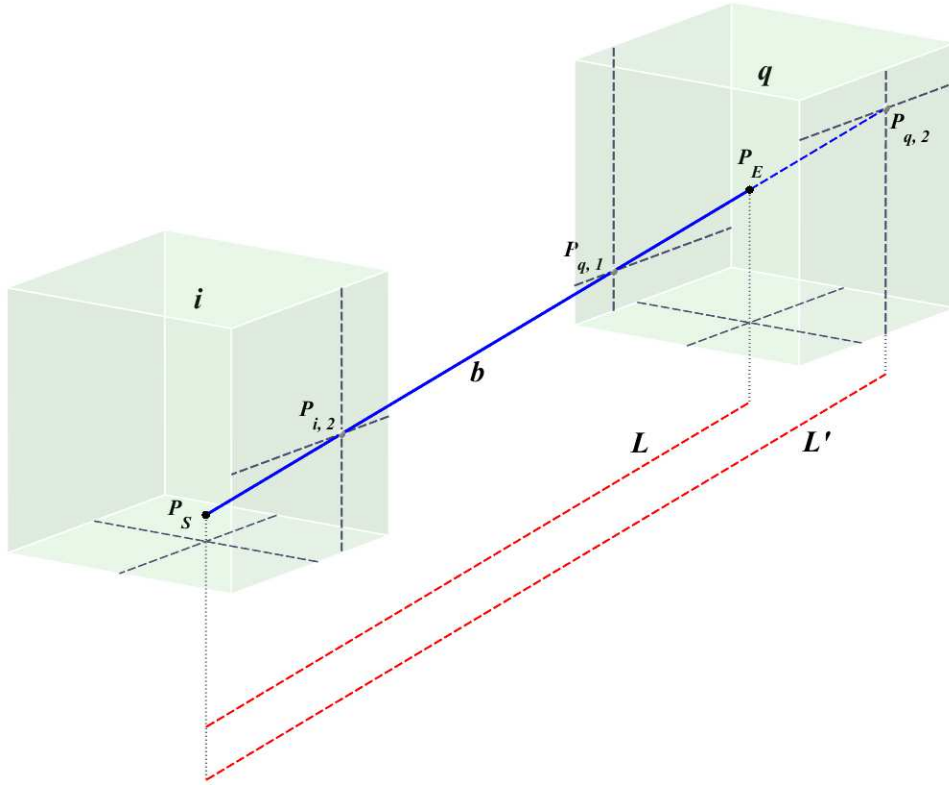


Figure 4.19: Entire macro-segment  $b$  and the two parent elements ( $i, q$ ) embedding its first  $(\mathbf{P}_S, \mathbf{P}_{i,2})$  and last  $(\mathbf{P}_{q,1}, \mathbf{P}_E)$  segment in Cartesian space. In dashed red, the given bar length ( $L$ ) and the accumulated length of tracked embedded segments ( $L'$ )

#### 4.3.4 Treatment of pyramid apex

When resorting to pyramidal elements to discretise the concrete bulk, additional provisions must be adopted to accommodate the possibility of a segment entering such parent element through its apex (node of intersection of the 4 triangular faces). In that specific node the transformation Jacobian becomes systematically singular, and consequently  $\bar{\mathbf{J}}_{\text{apex}}$  becomes undefined. This issue not only affects the dot product checks as per (4.17) but also prevents the first linearisation  $LI$  to be carried out following (4.19), and hence a segment such as the one depicted in Figure 4.20a could not be tracked.

A possible circumvention of this drawback consists of splitting the original pyramidal parent element into two tetrahedral elements of the same order (Figure 4.20b), which does not compromise conformity. Since tetrahedral elements retain Jacobian regularity in the entire domain enclosed by them (provided usual rules to avoid excessive distortion are complied with), the original pyramid apex becomes a regular tetrahedral node from where to start the linearising procedure described in Section 4.3.3.2 (Figure 4.20c).

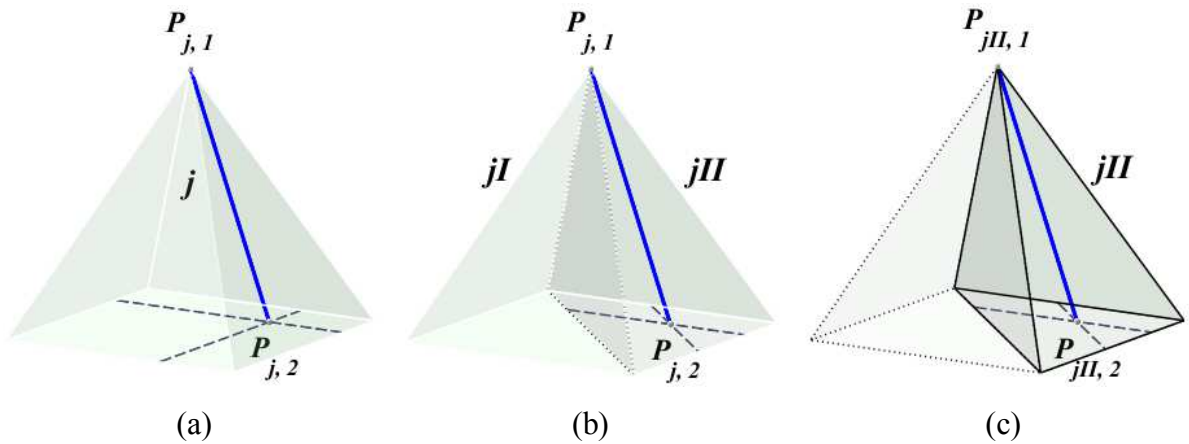


Figure 4.20: (a) Pyramidal parent element  $j$  with entry point of embedded segment located at the apex (b) Split of pyramidal parent element into two tetrahedral elements  $jI$  and  $jII$   
 (c) Admissible tetrahedral element  $jII$  as framework for initial linearisation

Although Figure 4.20 shows elements in Cartesian space, it is worth recalling that strictly speaking linearisations take place in the intrinsic coordinate space of the parent element. Hence, and following the example of Figure 4.20, changing the framework from original element  $j$  to element  $jII$  implies different coordinate spaces. After the first linearization  $LI$ , however, it is convenient to return to the pyramid parent element framework and track the

exit point  $\mathbf{P}_{j,2}$  within it, the reason being related to adjacency considerations. Neither of the tetrahedral elements  $(jI, jII)$  is properly defined in the concrete mesh as such (there is even the need of including an auxiliary dummy node in the diagonal edge across the pyramid square base), which in turn means that adjacency to the (fictitious) face separating the 2 tetrahedral elements is not defined. This can potentially become an issue if the original geometry is sufficiently distorted for the embedded segment to exit one tetrahedral element and enter the other through the common (fictitious) face.

Thus, for the second linearisation onwards, the change of coordinate space must start from

$$\begin{aligned}\mathbf{P}_{k,L1}^{PE} &= \left( \hat{\xi} \right)_{k,1}^{tet} + \Delta \hat{\xi}_{L1}^{tet} \\ \mathbf{P}_{k,L1}^b &= \mathbf{P}_{k,1} + \Delta \alpha_{\min}^{tet} \mathbf{d}_{SE}\end{aligned}\tag{4.33}$$

where Cartesian coordinates  $\mathbf{P}_{k,L1}^b$  must then be converted to pyramid element intrinsic coordinates via Inverse Mapping, allowing to continue as

$$\begin{aligned}\mathbf{P}_{k,Lj}^{PE} &= \left( \hat{\xi} \right)_{k,L(j-1)}^{b,pyr} + \Delta \hat{\xi}_{Lj}^{pyr} \\ \mathbf{P}_{k,Lj}^b &= \mathbf{P}_{k,L(j-1)}^b + \Delta \alpha_{\min}^{pyr} \mathbf{d}_{SE}\end{aligned}\tag{4.34}$$

for  $j \geq 2$ .

## 4.4 Contributions to stiffness and nodal forces

Although not explicitly stated in Section 4.2, the underlying assumption is that of perfect bond between reinforcing steel and surrounding concrete, since the degrees of freedom that the axial deformation of a given bar segment refers to are precisely the nodal ones of the embedding parent element. Bond slip, or even transverse segment deformation (‘dowel action’) could be accommodated for by adding the appropriate degrees of freedom, which would increase the order of the system, but otherwise proceeding in a formally identical manner to this section.

### 4.4.1 Segment axial deformation

The axial deformation  $\varepsilon_L$  in a given point  $P$  along the segment  $b$  embedded in a certain parent element is obtained by projecting the concrete strain tensor components  $\boldsymbol{\varepsilon}$  in the segment axial direction, formally equivalent to a change of base, from the original Cartesian

coordinate system  $(X, Y, Z)$  to another orthonormal system  $(X', Y', Z')$  where  $X'$  is aligned with the segment. In its most compact form, the axial deformation at  $P$  can be expressed as:

$$\epsilon_{L,P}^b = \frac{\partial \mathbf{d}_P}{\partial s} \cdot \mathbf{d}_{SE} \quad (4.35)$$

where  $\mathbf{d}_P = \{u, v, w\}_P^t$  stands for the global displacements of point  $P$  and  $s$  represents the Cartesian axial coordinate of the segment. Equation (4.35) stems from considering the linear strain tensor at point  $P$ :

$$(\epsilon_{ij})_P = \frac{1}{2} (\mathbf{d}_{i,j} + \mathbf{d}_{j,i})_P \quad (4.36)$$

under a change of base to a system where  $X' \triangleq s$ . Further elaboration of (4.35) by substituting displacements with their interpolation leads to:

$$\epsilon_{L,P}^b = \left( \begin{bmatrix} \frac{\partial \mathbf{N}}{\partial s} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \frac{\partial \mathbf{N}}{\partial s} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \frac{\partial \mathbf{N}}{\partial s} \end{bmatrix}_P \cdot \begin{Bmatrix} \mathbf{U} \\ \mathbf{V} \\ \mathbf{W} \end{Bmatrix} \right)^T \cdot \begin{Bmatrix} l_1 \\ m_1 \\ n_1 \end{Bmatrix} = \left\{ \left( \frac{\partial \mathbf{N}^\alpha}{\partial s} \right)_P \mathbf{U}_\alpha, \left( \frac{\partial \mathbf{N}^\alpha}{\partial s} \right)_P \mathbf{V}_\alpha, \left( \frac{\partial \mathbf{N}^\alpha}{\partial s} \right)_P \mathbf{W}_\alpha \right\} \cdot \begin{Bmatrix} l_1 \\ m_1 \\ n_1 \end{Bmatrix} \quad (4.37)$$

with  $\mathbf{N}$  being identical to the geometry shape functions vector in (4.6), and  $\{\mathbf{U}, \mathbf{V}, \mathbf{W}\}$  being the global displacement vectors of the parent element nodes. The repeated index  $\alpha$  implies summation and its range depends in turn on the element type. The intrinsic axial coordinate  $r$  is the counterpart of  $s$  in the segment intrinsic space (Figure 4.21) and relates to it via:

$$\frac{\partial r}{\partial s} = \frac{1}{|J_R^b|} = \frac{2}{L_R^b} \quad (4.38)$$

where  $\mathbf{J}_R$  is the transformation Jacobian between Cartesian coordinates and the intrinsic axial segment coordinate. The embedded segments are treated similar to a 3-noded 1D element with the intermediate node in the centre position, and hence determinant  $|J_R|$  equals half the segment length  $L_R$ . The directional derivatives of the parent element shape functions can be elaborated as:

$$\frac{\partial \mathbf{N}^a}{\partial s} = \frac{\partial \mathbf{N}^a}{\partial r} \cdot \frac{\partial r}{\partial s} = \left( \frac{\partial \mathbf{N}^a}{\partial \hat{\xi}_i} \frac{\partial \hat{\xi}_i}{\partial \hat{X}_j} \frac{\partial \hat{X}_j}{\partial r} \right) \cdot \frac{\partial r}{\partial s} = \left( \frac{\partial \mathbf{N}^a}{\partial \hat{\xi}_i} \right)^T \cdot \bar{\mathbf{J}} \cdot \mathbf{d}_{SE} \quad (4.39)$$

with  $\hat{\xi} = \{\zeta, \eta, \zeta\}^T$  and  $\hat{X} = \{X, Y, Z\}^T$ . Both indexes  $i$  and  $j$  imply summation. Substitution of (4.39) into (4.37) renders the more usual expression for the axial deformation at  $P$ :

$$\varepsilon_{L,P}^b = \frac{1}{|J_R|^2} \left[ \left( \frac{\partial \hat{X}}{\partial r} \otimes \frac{\partial \hat{X}}{\partial r} \right) \cdot \bar{\mathbf{J}} \cdot \frac{\partial \mathbf{N}^a}{\partial \hat{\xi}_i} \right]_P^T \cdot \begin{Bmatrix} u \\ v \\ w \end{Bmatrix}_a \quad (4.40)$$

originally derived in Ranjbaran (1996) for geometrically linear analysis.

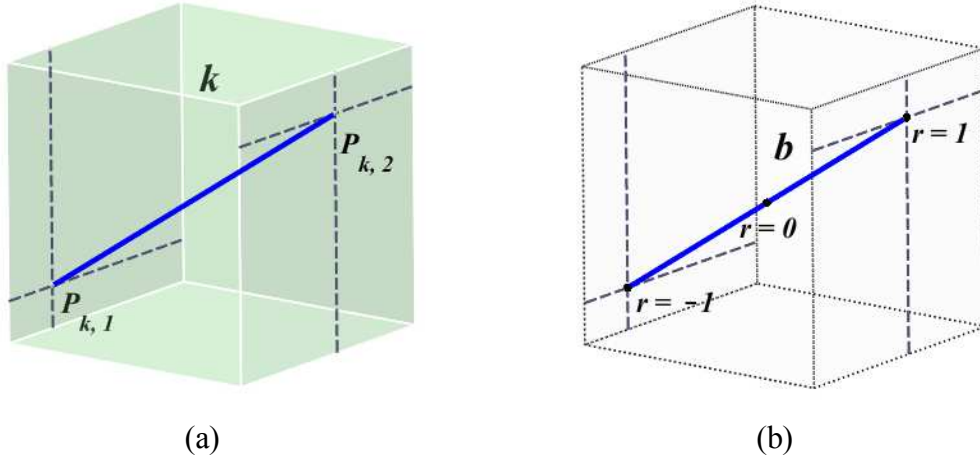


Figure 4.21: Embedded segment of bar  $b$  in parent element  $k$ , in (a) Cartesian coordinate space (b) segment intrinsic coordinate space

In order to account for geometric nonlinearity, the Green strain tensor at  $P$  must be considered instead of the linear strain tensor (4.36):

$$(\varepsilon_{ij})_P = \frac{1}{2} (\mathbf{d}_{i,j} + \mathbf{d}_{j,i} + \mathbf{d}_{k,i} \mathbf{d}_{k,j})_P \quad (4.41)$$

where index  $k$  implies summation. The same change of base that renders (4.35) from (4.36), if applied to (4.41), leads to:

$$\varepsilon_{L,P}^b = \frac{\partial \mathbf{d}_P}{\partial s} \cdot \left( \mathbf{d}_{SE} + \frac{1}{2} \frac{\partial \mathbf{d}_P}{\partial s} \right) \quad (4.42)$$

Analogously to (4.40), substitution of displacements with their interpolation can be finally elaborated as:

$$\varepsilon_{L,P}^b = \underbrace{\frac{1}{|J_R|^2} \left[ \left( \frac{\partial \hat{\mathbf{X}}}{\partial r} \otimes \frac{\partial \hat{\mathbf{X}}}{\partial r} \right) \cdot \bar{\mathbf{J}} \cdot \frac{\partial \mathbf{N}^\alpha}{\partial \hat{\xi}_i} \right]_P^T \cdot \begin{Bmatrix} u \\ v \\ w \end{Bmatrix}_\alpha}_{\text{linear}} + \underbrace{\frac{1}{2} \left[ \left( \frac{\partial \mathbf{N}^\alpha}{\partial \hat{\xi}_i} \right)^T \cdot \bar{\mathbf{J}} \cdot \mathbf{d}_{SE} \right]_P \cdot \begin{Bmatrix} u \\ v \\ w \end{Bmatrix}_\alpha}_{\text{quadratic supplement}}^2 \quad (4.43)$$

#### 4.4.2 Constitutive law for reinforcing steel

The stress evaluation at any given point  $P$  of an embedded bar segment requires the definition of a uniaxial material model as a function of the total axial strain (4.43). In the present work an elastic-plastic stress-strain law with linear hardening has been adopted, although generalisation to more sophisticated material curves could be accommodated with ease, without inducing any formal changes to the steps described in subsequent sections.

As with the strain tensor in the concrete parent elements (Chapter 3), the axial strain of the embedded segment can be split into an elastic and a plastic contribution, and hence the axial stress at point  $P$  of the segment pertaining to bar  $b$  can be expressed as:

$$\sigma_{L,P}^b = E \left( \varepsilon - \varepsilon_{\text{pl}} \right)_{L,P}^b \quad (4.44)$$

Similar to function (3.5) for concrete, all admissible stress states at a given segment point can be described here by the yield function:

$$f_{\text{pl}} = \sigma_{L,P}^b - \sigma_Y \leq 0 \quad (4.45)$$

with the linear hardening law:

$$\sigma_Y = \sigma_0 + H \left( \varepsilon_{\text{pl}} \right)_{L,P}^b \quad (4.46)$$

fully described with the yield stress  $\sigma_0$  and the constant plastic hardening modulus  $H$ . In this case the identification of the axial plastic strains with the equivalent strain  $\kappa_p$  in the full three-dimensional formulation is immediate (with  $H$  playing the role of  $\frac{\partial f_p}{\partial \kappa_p}$ ). The

tangential constitutive operator  $\theta_P^b = \left( \frac{\partial \sigma}{\partial \varepsilon} \right)_{L,P}^b$  becomes a scalar in this framework, and it can

be schematically visualised in Figure 4.22, where simple geometric arguments lead to:

$$\theta_P^b = \begin{cases} E & \text{if } \left( \dot{\varepsilon}_{\text{pl}} \right)_{L,P}^b = 0 \\ \frac{E \cdot H}{E + H} & \text{if } \left( \dot{\varepsilon}_{\text{pl}} \right)_{L,P}^b > 0 \end{cases} \quad (4.47)$$

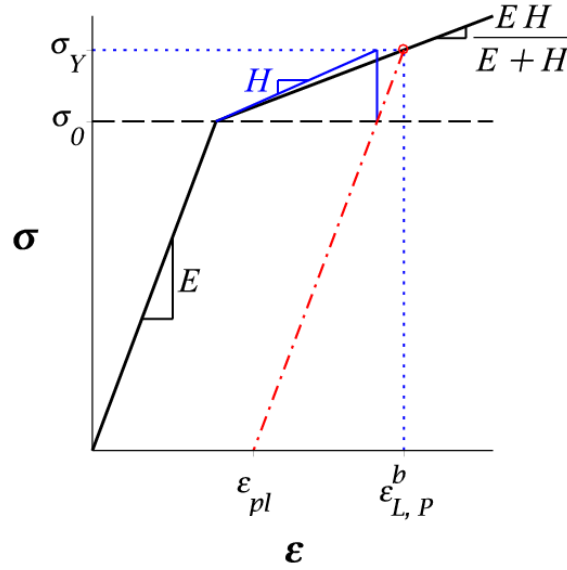


Figure 4.22: Material response of any macro-segment: elastic-plastic with linear isotropic hardening given by plastic hardening modulus  $H$

#### 4.4.3 Contribution at parent element level

Since the equilibrium of the mesh is formulated in weak form and no other strain components apart from the axial one are considered for the contribution of a segment to its embedding parent element, the corresponding term in the virtual work equation is:

$$\int_{V^b} \delta \varepsilon_L^b \sigma_L^b dV^b \quad (4.48)$$

for every embedded bar. All terms involved in the integral are scalars stemming from (4.43) and (4.44). Moreover, the virtual axial strain can be expressed as:

$$\delta \varepsilon_L^b = \frac{\partial \varepsilon_L^b}{\partial \mathbf{d}} \cdot \delta \mathbf{d} \quad (4.49)$$

with  $\mathbf{d}$  standing for global displacements. In the most generic case, including the effect of geometric non-linearity, it is the axial strain (4.43) that undergoes differentiation in (4.49), reading:

$$\frac{\partial \varepsilon_L^b}{\partial \mathbf{d}} = \frac{\partial}{\partial \mathbf{d}} \left( \frac{\partial \mathbf{d}_P}{\partial s} \cdot \left( \mathbf{d}_{SE} + \frac{1}{2} \frac{\partial \mathbf{d}_P}{\partial s} \right) \right) \quad (4.50)$$

Resorting to the *discretised* form of (4.50),  $\mathbf{d}$  then represents the global displacements of the relevant parent element nodes  $\left( \mathbf{d}_i = \{u_i, v_i, w_i\}^T \right)$ , and  $\mathbf{d}_P$  the interpolated displacement fields

within such parent element. After some elaboration, the discretised counterpart of (4.50) can be obtained as:

$$\frac{\partial \mathcal{E}_L^b}{\partial \mathbf{d}} = \left( \mathbf{d}_{SE} + \frac{\partial \mathbf{d}_P}{\partial s} \right) \frac{\partial \mathbf{N}^a}{\partial s} = \left( \mathbf{d}_{SE} + \frac{\partial \mathbf{N}^j}{\partial s} \mathbf{d}_j \right) \frac{\partial \mathbf{N}^a}{\partial s} \quad (4.51)$$

where the index  $j$  implies summation over all element nodes. Substitution of (4.51) in (4.49), and then in turn back in (4.48) considering that the discretised form of equilibrium via virtual work must be satisfied for any arbitrary  $\delta \mathbf{d}$ , leads to the following contribution to the nodal force vector of the bar ( $b$ ) segment embedded in parent element  $k$ :

$$\mathbf{F}_{(k)}^b = \int_{V^b} \frac{\partial \mathcal{E}_L^b}{\partial \mathbf{d}} \sigma_L^b dV^b \quad (4.52)$$

Performing integration (4.52) numerically along the segment axis via a Gauss-Legendre quadrature scheme gives rise to the final expression of the sought contribution:

$$\mathbf{F}_{(k)}^b = \sum_{gp=1}^{ngsl} \left( \frac{\partial \mathcal{E}_{L,gp}^b}{\partial \mathbf{d}} \sigma_{L,gp}^b A^b |J_R| W_{gp} \right) \quad (4.53)$$

where  $ngsl$  is the number of Gauss points considered along the segment axis, initially located with intrinsic axial coordinate  $r_{gp}$ , then translated to Cartesian space via:

$$\hat{\mathbf{X}}_{gp} = r_{gp} |J_R| \mathbf{d}_{SE} + \frac{1}{2} (\hat{\mathbf{X}}_{k,1} + \hat{\mathbf{X}}_{k,2}) \quad (4.54)$$

and finally transformed to parent element  $k$  intrinsic coordinates by means of Inverse Mapping. In (4.53),  $A^b$  stands for the cross-sectional area of the segment, assumed constant throughout the bar, and  $W_{gp}$  is the Gauss weight function associated to Gauss point  $gp$ , whence the last triplet in the summation term can be seen as a Gauss volume.

In order to obtain the contribution to the parent element stiffness matrix, differentiation of (4.52) is required:

$$\mathbf{K}_{(k)}^b = \frac{\partial \mathbf{F}_{(k)}^b}{\partial \mathbf{d}} = \int_{V^b} \frac{\partial \mathcal{E}_L^b}{\partial \mathbf{d}} \frac{\partial \sigma_L^b}{\partial \mathbf{d}} dV^b + \int_{V^b} \frac{\partial^2 \mathcal{E}_L^b}{\partial \mathbf{d} \partial \mathbf{d}} \sigma_L^b dV^b \quad (4.55)$$

The first summand in (4.55) relates to the material response whilst the second arises from the inclusion of geometric non-linearity in (4.43). Elaborating the integrands separately:

$$\frac{\partial \varepsilon_L^b}{\partial \mathbf{d}} \frac{\partial \sigma_L^b}{\partial \mathbf{d}} = \frac{\partial \varepsilon_L^b}{\partial \mathbf{d}} \frac{\partial \sigma_L^b}{\partial \varepsilon_L^b} \frac{\partial \varepsilon_L^b}{\partial \mathbf{d}} = \frac{\partial \varepsilon_L^b}{\partial \mathbf{d}} \theta^b \frac{\partial \varepsilon_L^b}{\partial \mathbf{d}} \quad (4.56)$$

with  $\theta^b$  as obtained in (4.47), and:

$$\frac{\partial^2 \varepsilon_L^b}{\partial \mathbf{d} \partial \mathbf{d}} = \frac{\partial}{\partial \mathbf{d}} \left( \mathbf{d}_{SE} \frac{\partial \mathbf{N}^a}{\partial s} + \frac{\partial \mathbf{N}^j}{\partial s} \mathbf{d}_j \frac{\partial \mathbf{N}^a}{\partial s} \right) = \frac{\partial}{\partial \mathbf{d}} \left( \frac{\partial \mathbf{N}^j}{\partial s} \mathbf{d}_j \frac{\partial \mathbf{N}^a}{\partial s} \right) \quad (4.57)$$

which evolves into a matrix comprising exclusively diagonal 3x3 blocks, as differentiation in (4.57) can only be non-zero when performing it with respect to  $\mathbf{d}_j$ . Hence, the structure of any block reads:

$$\left( \frac{\partial^2 \varepsilon_L^b}{\partial \mathbf{d} \partial \mathbf{d}} \right)_{IJ} = \begin{pmatrix} \frac{\partial \mathbf{N}^I}{\partial s} \frac{\partial \mathbf{N}^J}{\partial s} & 0 & 0 \\ 0 & \frac{\partial \mathbf{N}^I}{\partial s} \frac{\partial \mathbf{N}^J}{\partial s} & 0 \\ 0 & 0 & \frac{\partial \mathbf{N}^I}{\partial s} \frac{\partial \mathbf{N}^J}{\partial s} \end{pmatrix} \quad (4.58)$$

where the range of  $I$  and  $J$  depends on the element type. Applying elaborations (4.56) - (4.58) to (4.55), along with the Gauss-Legendre quadrature scheme for numerical integration, provides the expression to compute the contribution to the parent element  $k$  stiffness matrix of bar  $b$ :

$$\mathbf{K}_{(k)}^b = \sum_{gp=1}^{ngsl} \left( \frac{\partial \varepsilon_{L,gp}^b}{\partial \mathbf{d}} \theta_{gp}^b \frac{\partial \varepsilon_{L,gp}^b}{\partial \mathbf{d}} A^b |J_R| W_{gp} \right) + \sum_{gp=1}^{ngsl} \left( \frac{\partial^2 \varepsilon_{L,gp}^b}{\partial \mathbf{d} \partial \mathbf{d}} \sigma_{L,gp}^b A^b |J_R| W_{gp} \right) \quad (4.59)$$

#### 4.4.4 Potential extension of the model to account for material overlapping

As presented in Huber (2006), and elaborated in Gebbeken (1996) for composite materials, the Rebar model applied to reinforced concrete accounts for the fact that material points along an embedded segment are hitherto linked to both constituents simultaneously, hence contributing twice to the total element stiffness matrix and nodal force vector.

Although this issue does not bear significance for moderate to low reinforcement ratios, it may do so for dense reinforcement arrangements. Hence, in such situations the segment contributions (4.53) and (4.59), carried out in the intrinsic axial coordinate space of the segment, would have to evolve parallel to the calculation of the parent element integral along the same axis. In the framework of the Rebar model, this contribution of concrete points

along the segment axis should be subtracted from the total element stiffness matrix. This approach, however, has limitations, since the steel bars are not treated as 3D solids associated to a triaxial material model. As shown in Section 4.4.2, each segment is discretised with 1D elements, the stiffness of which consists solely of axial components. Hence, upon sufficient mesh refinement, the situation could arise where a parent element would lose significant transverse stiffness when subtracting the contribution of the embedded bar segment(s). Since all segments are modelled with purely axial elements, there would be no steel transverse stiffness replacing the subtracted concrete equivalent. A potential remedy to this whilst keeping the 1D character of the elements modelling the reinforcement would be to extend its formulation to include transverse stiffness ('dowel effect').

Additionally, and following the original Rebar model formulation, the *negative* contribution of concrete along the segment axis, under the same quadrature scheme as the segment, would read:

$$\mathbf{F}_{(k)}^{b,C} = - \int_{-1}^1 \mathbf{B}^t \boldsymbol{\sigma} A^b |J_R| dr \simeq - \sum_{gp=1}^{ngs1} \left( \mathbf{B}_{gp}' \boldsymbol{\sigma}_{gp} A^b |J_R| W_{gp} \right) \quad (4.60)$$

$$\mathbf{K}_{(k)}^{b,C} = - \int_{-1}^1 \mathbf{B}^t \boldsymbol{\Theta} \mathbf{B} A^b |J_R| dr = - \sum_{gp=1}^{ngs1} \left( \mathbf{B}_{gp}' \boldsymbol{\Theta}_{gp} \mathbf{B}_{gp} A^b |J_R| W_{gp} \right) \quad (4.61)$$

for the nodal force vector and element stiffness matrix respectively, with nominal stresses  $\boldsymbol{\sigma}$  and algorithmic tangential operator  $\boldsymbol{\Theta}$  computed as described in Chapter 3. From here, the nodal force vector and stiffness matrix of parent element  $k$  accounting for the *net* contribution of the embedded segment of bar  $b$  would be given as:

$$\mathbf{F}_{(k)} = \mathbf{F}_{(k)}^C + \left( \mathbf{F}_{(k)}^b + \mathbf{F}_{(k)}^{b,C} \right) \quad (4.62)$$

$$\mathbf{K}_{(k)} = \mathbf{K}_{(k)}^C + \left( \mathbf{K}_{(k)}^b + \mathbf{K}_{(k)}^{b,C} \right) \quad (4.63)$$

where the bracketed term in (4.62) and (4.63) can become in general a summation over all bar segments traversing parent element  $k$ . Although the concrete stress evaluation in the segment Gauss points as per (4.60)-(4.61) is feasible, it is not computationally efficient. Instead, it is considered more convenient to establish a mapping from the already evaluated stresses at the parent element Gauss points to the Gauss points of the embedded segment.

In light of these disquisitions, and the potential shortcomings of the original Rebar model, it is decided not to include it in the final implemented version of the constitutive model. The discussed remedies leading to an enhanced Rebar model, though not pursued in this Thesis, are desirable and expected to be elaborated in the future.

## 4.5 Control test

In order to verify the functionality of the reinforcement inclusion in the model, a simple control test is carried out, based on a single element under tensile loading. This test notionally follows Huber (2006), who in turn based his test on Gebbeken (1996), though for different dimensions and material parameters. The load  $q$  is applied uniformly on the top face of a prismatic hexahedral element of length  $L = b = 0.5$  m, with fixity restraints applied on all nodes of the opposite face. Both loading and boundary conditions are shown in Figure 4.23, where a specific node is marked as reference for displacement tracking in the direction of loading. Four different options for reinforcement arrangement are considered altogether, based on 32 mm bar diameter throughout.

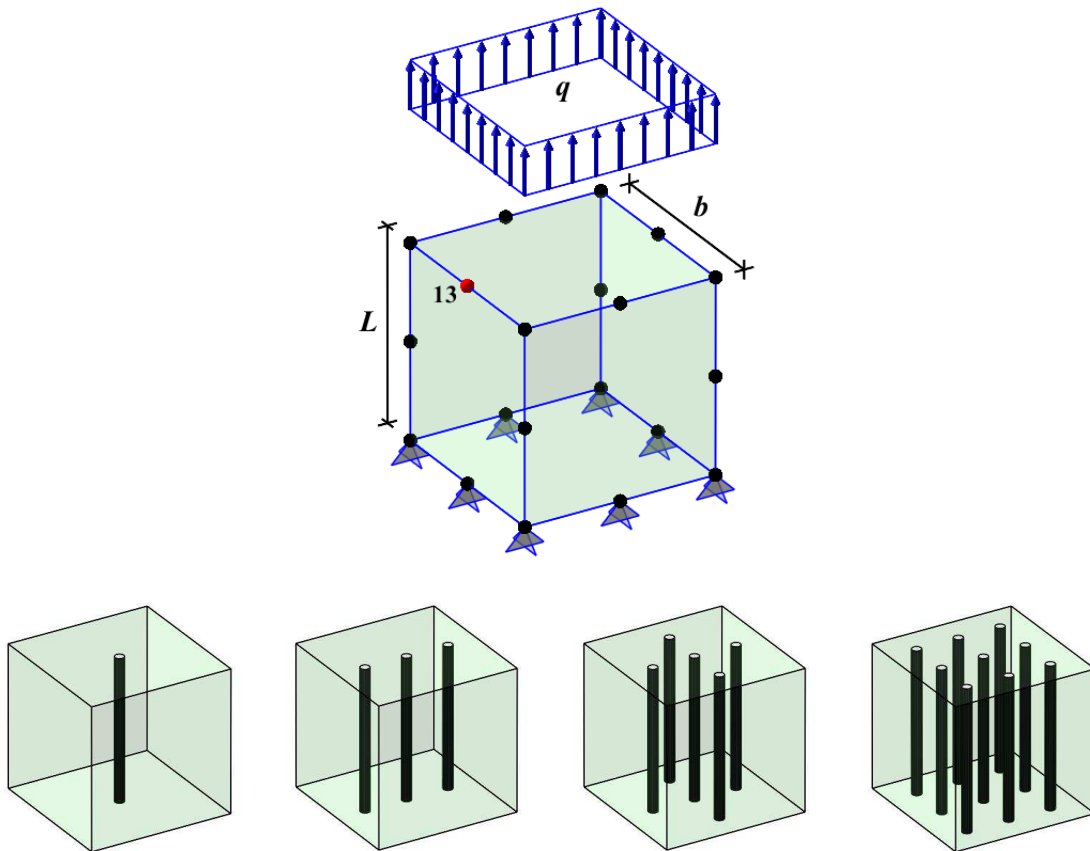


Figure 4.23: (top) Tensile control test on a single hexahedral element, with the node to track displacements highlighted in red (bottom) Reinforcement arrangements with H32 bars

In all arrangements, shown also in Figure 4.23, the bars are oriented following the direction of loading, giving rise to the following reinforcement ratios:

$$\begin{aligned} 1H32 &\rightarrow \rho \approx 0.32\% \\ 3H32 &\rightarrow \rho \approx 0.96\% \\ 5H32 &\rightarrow \rho \approx 1.61\% \\ 9H32 &\rightarrow \rho \approx 2.89\% \end{aligned}$$

These values of reinforcement ratio relate to the concrete gross cross-section  $A_c^g$ , and do not change significantly if related to the net cross-section given their low range. The adopted material parameters are:

$$\begin{array}{l} \text{concrete} \left\{ \begin{array}{l} E = 31000 \text{ MPa} \\ \nu = 0.2 \\ f_c = 30 \text{ MPa} \\ f_t = 2.4 \text{ MPa} \\ G_f = 70 \text{ J/m}^2 \end{array} \right. \quad \text{steel} \left\{ \begin{array}{l} E_s = 200000 \text{ MPa} \\ f_y = 400 \text{ MPa} \\ H = 20 \text{ MPa} \end{array} \right. \end{array}$$

Figure 4.24 shows the response curves for all reinforcement arrangements (including illustratively the curve corresponding to plain concrete), in terms of resultant force  $Q = qb^2$  against the vertical displacement of node 13. As expected, all curves end up stabilising at a progressively higher plateau level upon bar yielding, transitioning after cracking from the softening branch asymptotically towards the response of the unconfined steel bars.

As noted in Huber (2006), it is possible to derive an analytic expression for the axial displacement in uncracked state up to peak load by means of homogenising the concrete cross-section:

$$A_c^h = (1 - \rho_s) A_c^g + \frac{E_s}{E_c} A_s \quad (4.64)$$

to then obtain displacements prior to cracking as:

$$w_{13} = \frac{QL}{E_c A_c^h} \quad (4.65)$$

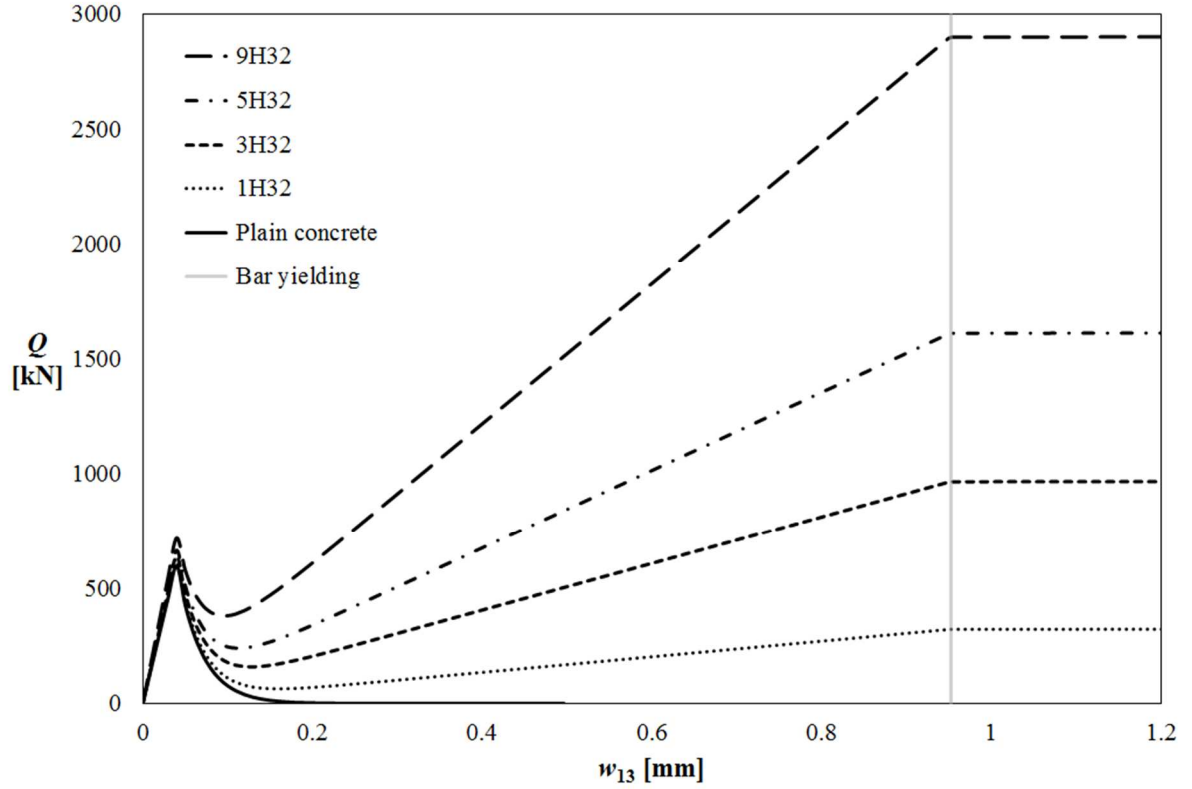


Figure 4.24: Response curve of the numerical control test for all reinforcement arrangements

Resorting to (4.65) for the extreme cases of 1H32 and 9H32 leads to displacement values at peak load of  $w_{13} = 0.039$  mm and  $w_{13} = 0.046$  mm respectively. As reference,  $w_{13} = 0.039$  mm corresponds to plain concrete. This range of displacements is reasonably reflected in the response curves resulting from the proposed reinforced concrete model, shown in Figure 4.24.

Since the induced strain field is homogeneous in the element, the characteristic element size parameter is chosen in this case to coincide with the actual hexahedron side length ( $h = 0.5$  m). If such element length along the bar is kept constant and the width  $b$  is considered as a free parameter for the case of a single central bar, the resulting parametric response curves change as per Figure 4.25.

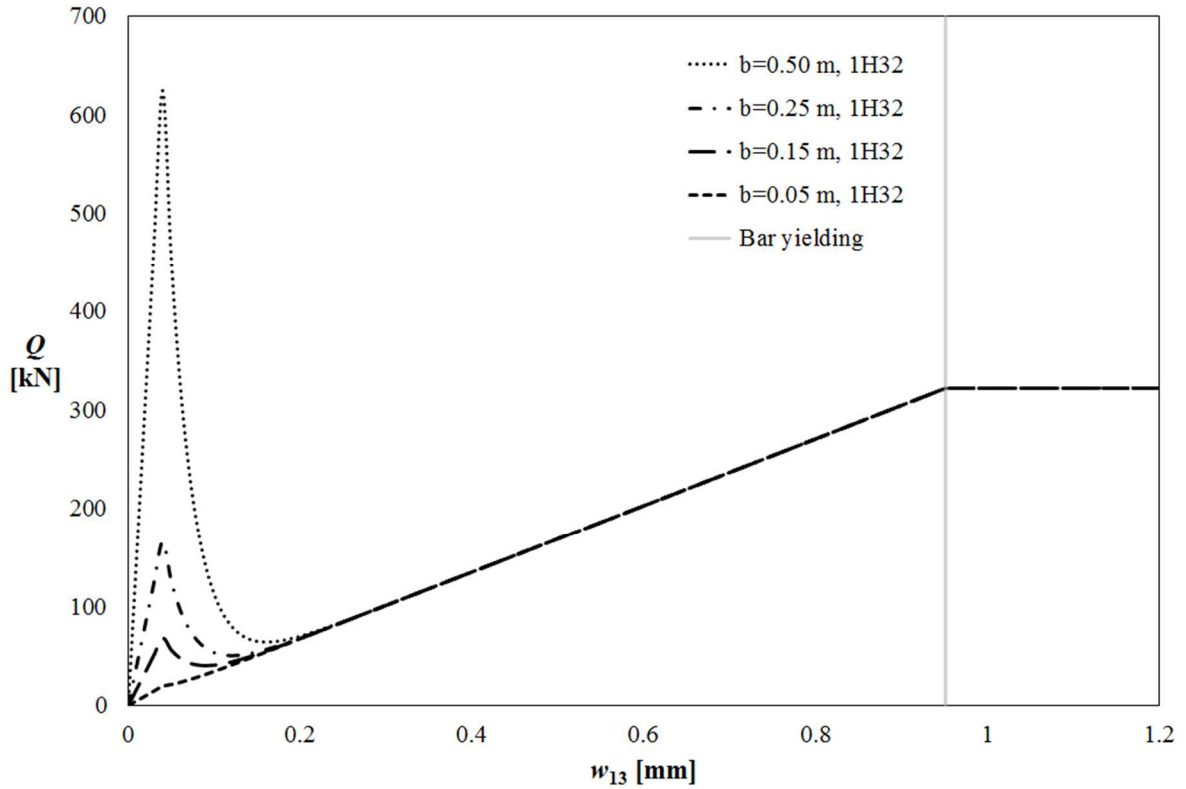


Figure 4.25: Parametric response curves of the control test for 1H32

The curve corresponding to  $b = 0.5$  m retrieves the one depicted in Figure 4.24. The area enclosed between this curve and the unconfined steel bar response represents the cumulative effect of the fracture energy over the whole cross section, i.e.  $G_f b^2$ . Such quadratic variance of enclosed area is correctly displayed by the curves of Figure 4.25. Assigning a smaller value to the characteristic element size  $h$  entails overestimating the fracture energy in this case, as the contribution of concrete would cease at greater values of displacement. In more generic cases of extensive meshes, however, modification of the characteristic element size estimated solely on projection may be necessary to achieve consistency with the fracture energy, as is discussed in Chapter 5.

## 4.6 Conclusions

The embedded approach for modelling of reinforcement is selected as the most suitable, based on its capability of allowing arbitrary bar orientation within a concrete parent element. Hence, the concrete element mesh arrangement can be guided by stress considerations, effectively decoupled from the reinforcement arrangement.

The algorithm presented and discussed in this chapter incorporates additional novel features that allow for an efficient and robust treatment of discretised embedded bars, from their location within an arbitrary concrete mesh to their sequential tracking up to their end point. Embedded segments are not approximated by its chord and retain their interpolated shape. The described procedures are approached systematically and are readily applicable to any parent element type and geometry, accommodating every potential source of ambiguity in the form of bars lying on shared parent element faces, edges or vertex nodes, including the singular case of a pyramid apex. The resulting bar discretisation is shown to be accurate, without resorting to simplifications applied in previous models, and can sustain parent element distortions within the usual bounds to maintain univocal relations between Cartesian and intrinsic coordinates.

The contribution of discretised embedded segments to their parent element stiffness matrix and nodal force vector is established, and the omission of an adjustment for the material overlap is justified. Implementation of these contributions along with the bar discretisation module into the nonlinear Finite Element software ADAPTIC (Izzuddin, 1991) allows for the simulation of reinforced concrete loading processes, as is presented in Chapter 5 for benchmark tests and in Chapter 6 for two major case studies.

# CHAPTER 5

## Numerical applications

### 5.1 Introduction

Following the material modelling description of the two main constituents, as well as their respective model verification (concrete in Chapter 3 and reinforcement in Chapter 4), the current chapter aims at validating these models via numerical simulations of various benchmark tests. Plain concrete is simulated in the framework of:

1. three-point bending,
2. torsion, and
3. mixed torsion-bending

of notched specimens, along with uniaxial compression of regular cubic and cylindrical specimens, whereas reinforced concrete is simulated via three point bending of unnotched specimens. The simulations are carried out with the nonlinear Finite Element software ADAPTIC v2.15.2 (Izzuddin, 1991). All three-dimensional elements used for mesh generation are of quadratic order with either full or reduced Gauss integration. Moreover, the elements belong to the Serendipity class, i.e. quadratic character is achieved using nodes only on the element edges.

Additional aspects of numerical nature, partly commented upon in Chapters 2-4, are investigated and assessed in their application to some of the aforementioned simulations. In all cases, it is resorted by default to static analysis with isotropic damage, full Gauss integration and no domain partitioning. Modifications of these options (e.g. dynamic analysis) or inclusion of additional analysis tools (e.g. localisation analysis) is duly noted where appropriate.

## 5.2 Three-point bending of notched specimen

In this test, performed originally by Kormeling and Reinhardt (1983), a 450 mm long concrete beam of square cross-section and a 5 mm wide notch across the bottom face width at midspan is subjected to a vertical knife edge load at the opposite side of the notch cross-section. The beam is simply supported and the notch extends up to half of the member depth, as shown in Figure 5.1. The out-of-plane width is 100 mm. Further descriptions of the experimental setup, along with the load application procedure, can be found in Kormeling and Reinhardt (1983).

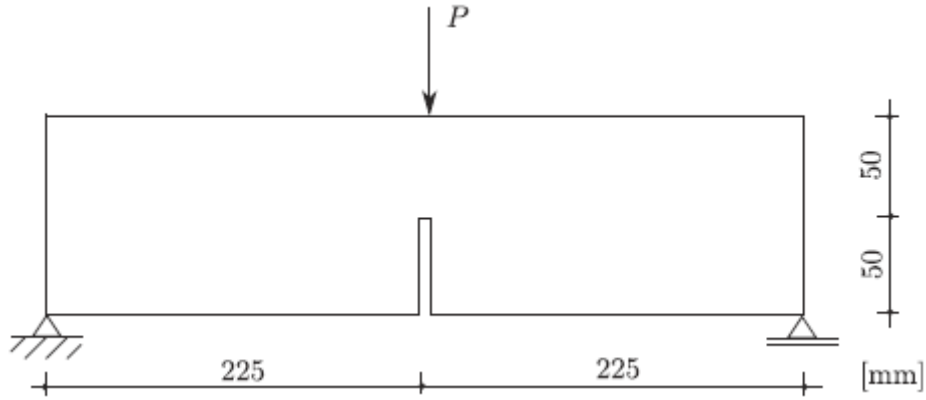


Figure 5.1: Geometry and experimental setup of the Kormeling and Reinhardt 3-point bending test (Grassl *et al.*, 2013)

Following simulations by Grassl *et al.* (2013), the material parameters are taken as:

$$E = 20000 \text{ MPa}$$

$$\nu = 0.2$$

$$\bar{f}_c = 24 \text{ MPa}$$

$$\bar{f}_t = 2.4 \text{ MPa}$$

$$G_f = 100 \text{ J/m}^2$$

As elaborated in Chapter 3, it is considered more computationally beneficial to treat the characteristic element size  $h$  representing the damage bandwidth as a fixed parameter. Since the region of the mesh where damage is expected to occur (i.e. the vicinity of the central notch) is fairly regular, this approach is deemed justified. Consequently, this additional parameter is taken as  $h = 2.5 \text{ mm}$ , considering that localisation may concentrate in a band thinner than the notch itself. For the simulation, a structured mesh consisting of 7288 20-node isoparametric hexahedrons is used, with a progressive reduction of element size along the

central body surrounding the notch, as shown in Figure 5.2. Qualitatively, the element size ranges between 30 mm in the outer corners and 5 mm in the vicinity of the notch.

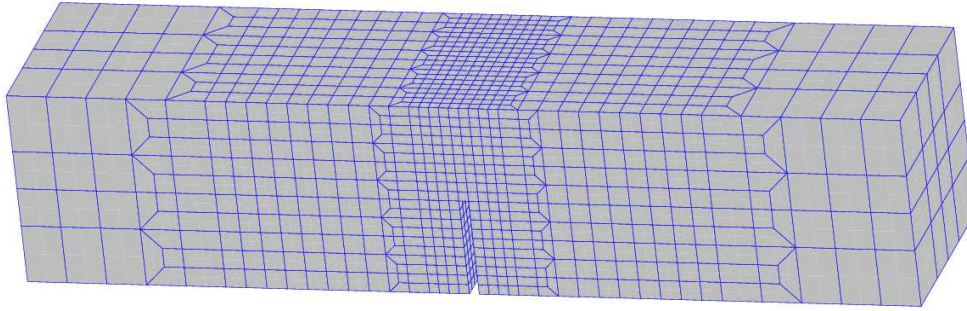


Figure 5.2: Mesh used for the three-point bending simulation

Figure 5.3 shows the load vs. crack-mouth-opening-displacement (CMOD) curve along with the experimental bounds as reported by Kormeling and Reinhardt (1983). The estimated peak load attains a value within the experimental bounds though closer to the maximum recorded value. Although the post-peak branch displays a less steep slope at onset of softening, it tends towards the experimental bounds with increasing displacement and remains stable throughout. The dissipated energy is slightly overestimated, though this stems from the adopted constant value of parameter  $h$ . Damage does indeed localise into a band narrower than the notch, but the effective bandwidth is greater than the assumed value of  $h$ . Overall, however, the global response is considered to be captured reasonably.

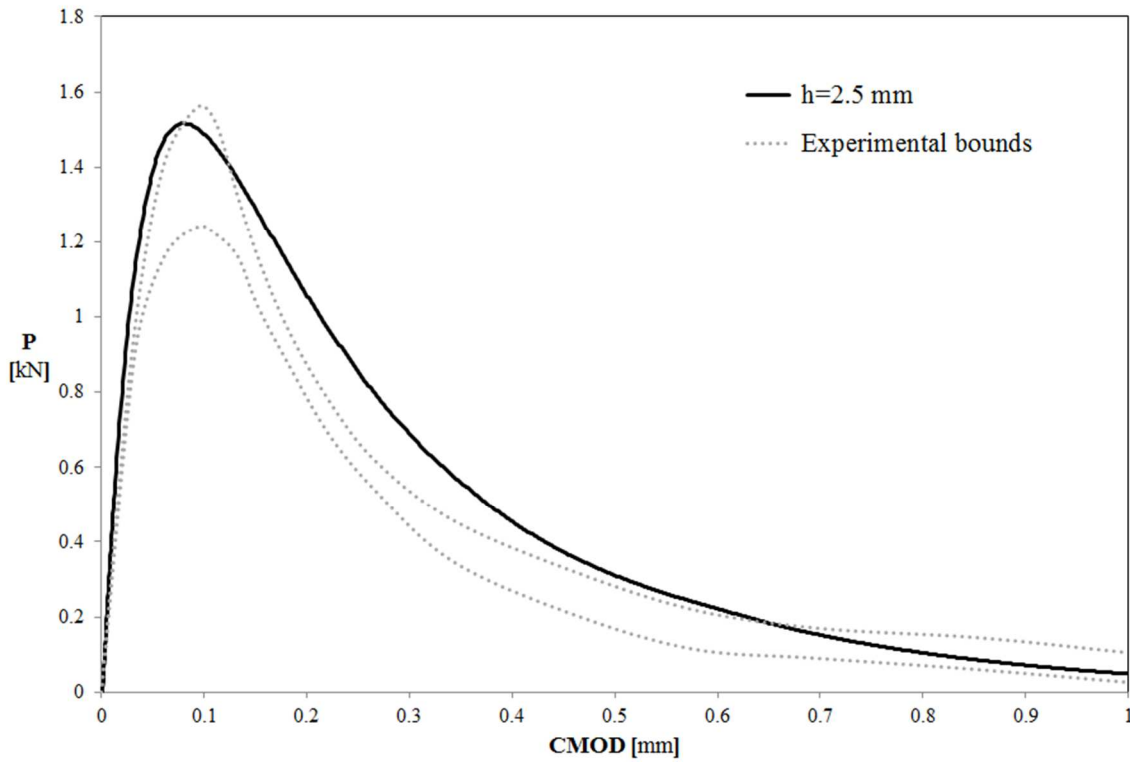


Figure 5.3: Load-CMOD curve and experimental scatter with  $h$  as fixed parameter

In this particular case, since the expected crack path is already aligned with the mesh orientation, there is no trace of directional bias. The evolution of damage along the plane of the notch is shown in Figure 5.4.

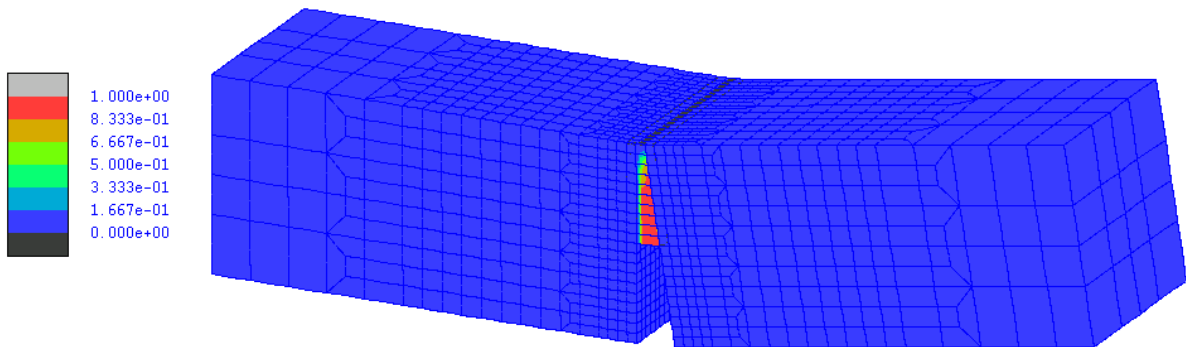


Figure 5.4: Scalar damage variable  $\omega$  distribution at post-peak (CMOD  $\sim$  1 mm), with deformations magnified by a factor of 20

### 5.2.1 Effect of calculated bandwidth

The same analysis as in the previous section is carried forward, with identical material properties, changing the character of  $h$  from fixed parameter to a function of the damage

orientation and element morphology, following the projection method by Govindjee *et al.* (1995) elaborated in Chapter 3. Exceptionally, analysis is carried out following a modified Newton scheme resorting to the secant stiffness  $(1-\omega)\mathbf{D}_e$  instead of a full Newton scheme with the elasto-plastic-damage algorithmic stiffness, favouring robustness over convergence rate.

As shown in Figure 5.5, the load vs. CMOD curve retains its shape and main features when compared to its counterpart in Figure 5.3. However, as anticipated in Chapter 3, projection methods do not account for localisation developing along a subset of Gauss points within a finite element, which is not irrelevant when resorting to higher order elements, as can be corroborated by the underestimation of energy dissipation in Figure 5.5. It is thus argued, following Slobbe *et al.* (2013), that a factor  $\gamma$  accounting for such possibility should affect the damage bandwidth estimator (3.122), bearing in mind that the same formal limitations as when fixing  $h$  as a parameter apply, i.e. the region of the mesh where damage is expected to occur should not be too irregular. By setting  $\gamma = 0.7$ , energy dissipation and peak load are estimated correctly, as shown in Figure 5.5.

In any case, and additionally to the drop in convergence rate from quadratic to linear when switching from a full to a modified Newton scheme, calculating  $h$  for every iteration at every Gauss point has a significant retarding effect on performance. This is observed even in a case like the current one, with a single crack plane already oriented parallel to one of the mesh main directions. Hence, since the computational benefits of calculating  $h$  do not overcome its potential drawbacks, it is decided not to apply this approach any further and predefine  $h$  as a fixed parameter for the rest of the numerical examples in this chapter as well as the major case studies of Chapter 6.

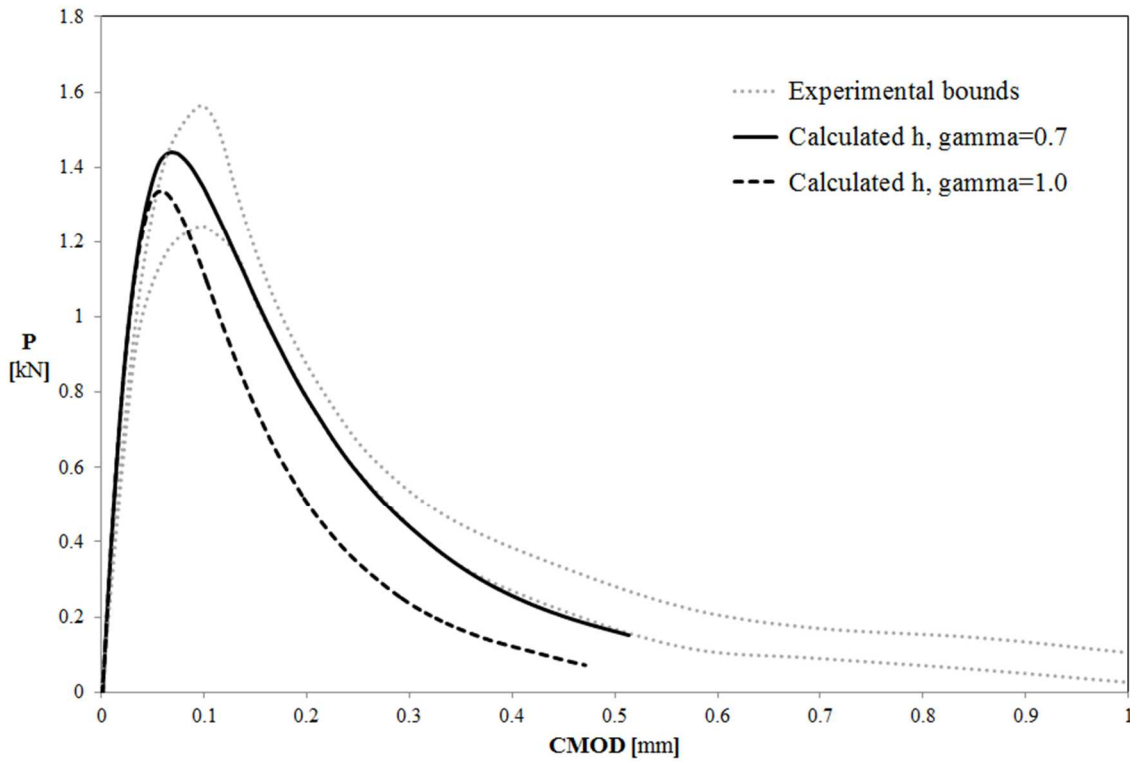


Figure 5.5: Load-CMOD curves calculating  $h$  for different  $\gamma$  values

### 5.3 Torsion beam

As described for instance by Jefferson and Bennett (2005), the Barr and Brokenshire torsion test consists of a 400 mm long concrete beam of square cross-section with a  $45^\circ$  skewed notch of 5 mm in width across the upper face and extending up to half of the beam depth. At its edges, the beam is supported by rigid steel legged frames. Such frames are arranged as clamps, and the vertical load applied on one of the steel legs combined with the resulting reactions on the other three legs provide for the torsion moment.

The geometry of all involved elements as well as the experimental setup are schematically shown in Figure 5.6, and a detailed description can be found in Barr and Brokenshire (1996).

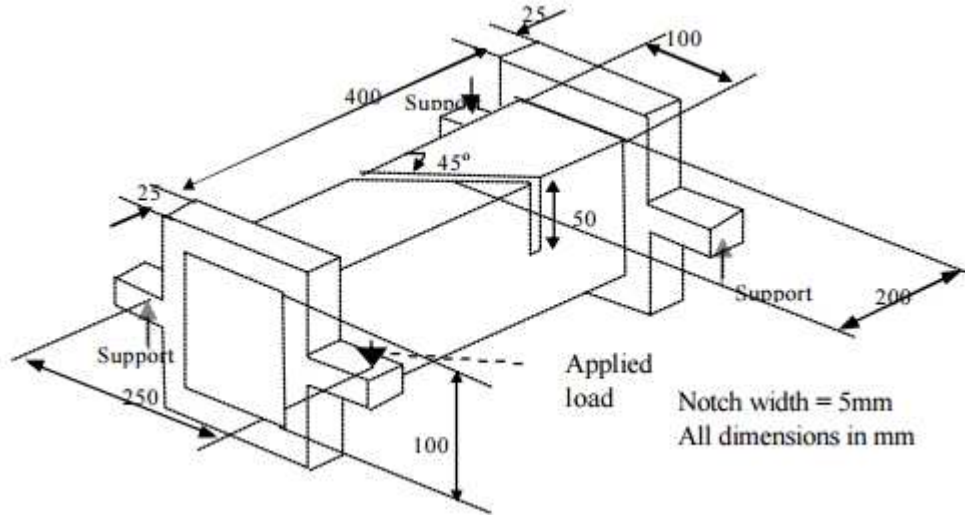


Figure 5.6: Geometry and experimental setup of the Barr and Brokenshire torsion test, from Jefferson and Bennett (2005)

The material parameters are taken from the reported values in the reference as follows:

$$E = 35000 \text{ MPa}$$

$$\nu = 0.2$$

$$\bar{f}_c = 40 \text{ MPa}$$

$$\bar{f}_t = 3 \text{ MPa}$$

$$G_f = 80 \text{ J/m}^2$$

Following Huber (2006), the steel frames have been simplified in the simulation to just the legs being attached to the artificially stiff concrete elements that would be clamped in reality. Since this modification does not affect the development of damage in the vicinity of the notch, which is the critical region, this is considered reasonable. In total, 996 20-node hexahedral elements form the structured mesh, whereby the element distribution is denser around the skewed notch (Figure 5.7). Analysis is governed throughout by direct displacement control of the load application node.

Since there is minor distortion in the mesh originating from the skewness of the notch plane with respect to the specimen cross-section, the choice of the additional fixed parameter  $h$  is less intuitive than in Section 5.2. To investigate the sensitivity of the response to the characteristic element size, a parametric study on this variable is performed.

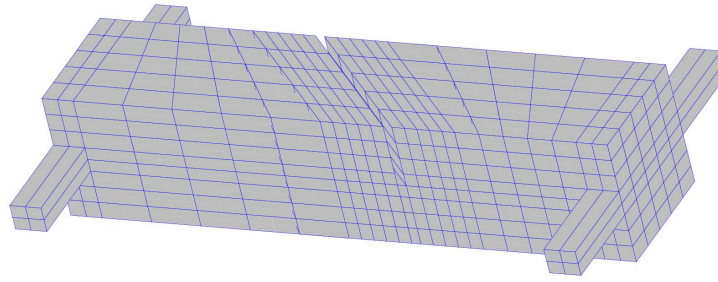


Figure 5.7: Mesh of 20-node hexahedrons used for the Barr and Brokenshire torsion test

In order to assess the output of the simulation, a comparison with the test results is made in terms of the load vs. crack-mouth-opening-displacement (CMOD, measured in the direction perpendicular to the notch plane at mid-width) curve. This is shown in Figure 5.8 for all values of  $h$  considered, along with the experimental scatter as per Jefferson and Bennett (2005).

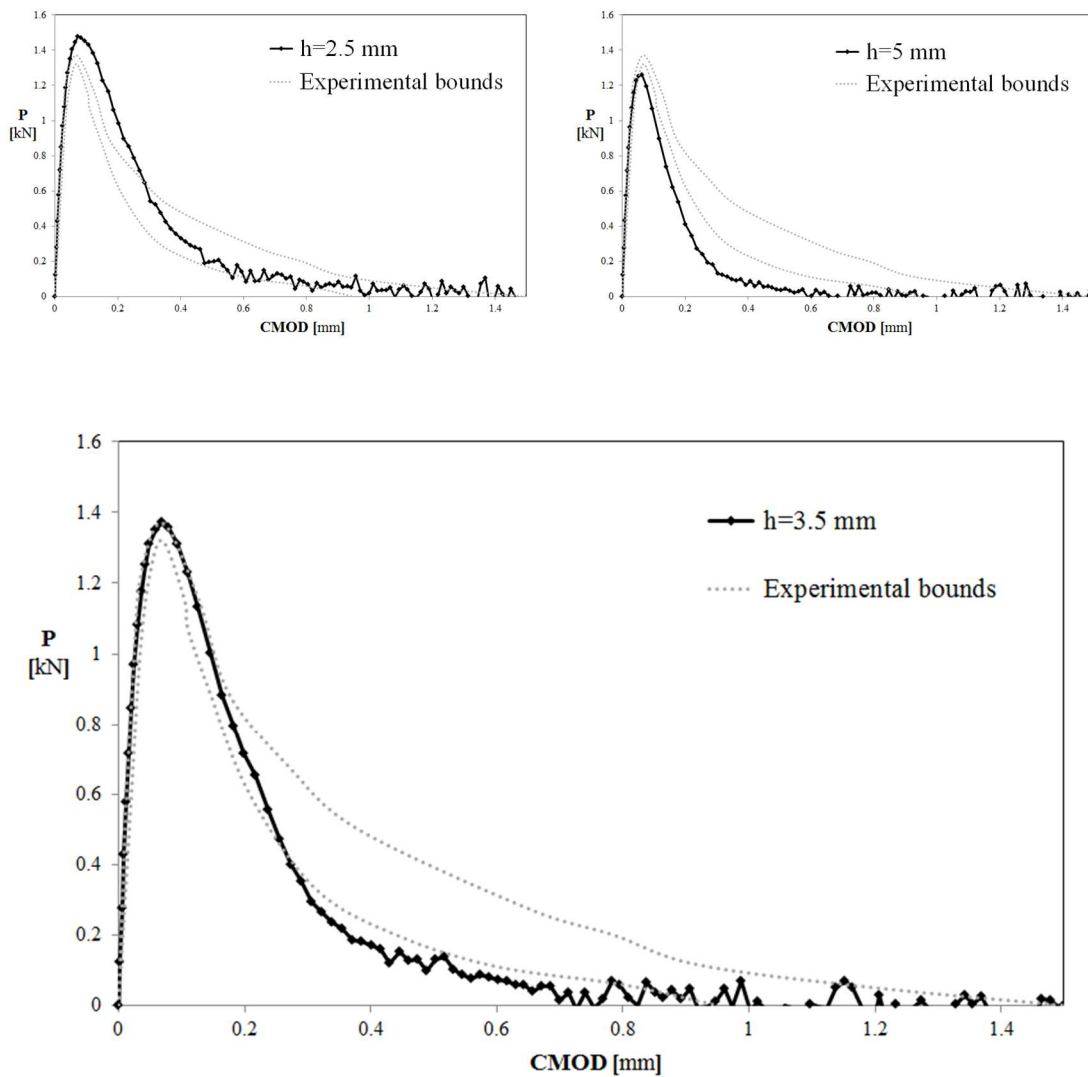


Figure 5.8: Load-CMOD curve for different values of  $h$

The highlighted curve in Figure 5.8 corresponds to  $h = 3.5$  mm and displays the best fit with the experimental peak load, although at the cost of being a lower bound for dissipated energy. This value of characteristic element size represents a damage bandwidth of 70% of the size of elements along the skewed notch width. The post-peak branch is tracked adequately, but an onset of instability triggered at advanced states of damage is recorded for all values of  $h$ . The underlying reason is thought to be related to either the mesh topology or the isotropic character of the scalar damage model, as for severely damaged states all components of the local stiffness associated to a sample point drop to zero proportionally. This is further investigated in Sections 5.3.1-5.3.3.

The crack surface observed in the experiment is not a plane but a complex curved surface anti-symmetric with respect to the centre of the notch tip (Figure 5.9). Hence, there is an apparent misalignment of the expected damage propagation direction and the mesh orientation. As a consequence of this misalignment, and anticipated in Chapter 3, the resulting crack pattern displays mesh induced directional bias. Figure 5.10 illustrates this issue by showing the damage distribution in an advanced post-peak state (CMOD of approximately 1.5 mm). It has an evident tendency to follow the plane of the notch, as it is in turn aligned with the mesh.

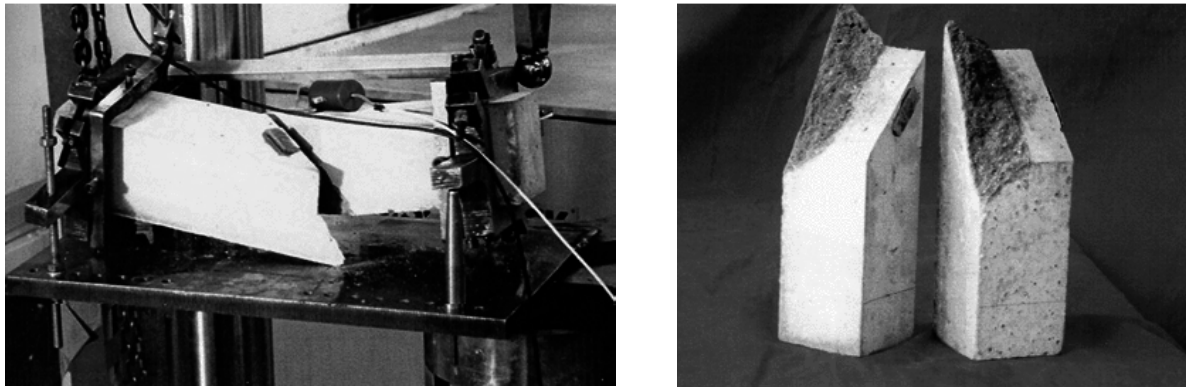
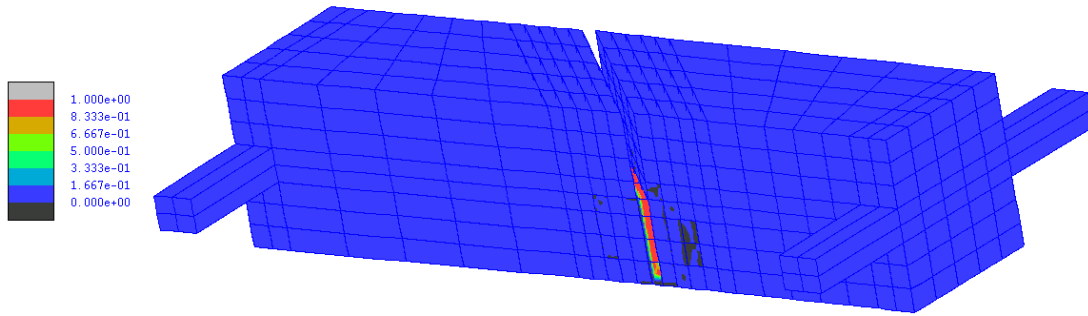


Figure 5.9: Torsion beam after failure and split specimen blocks (Barr and Brokenshire, 1996)

Figure 5.10: Damage variable  $\omega$  distribution at post-peak

In order to assess the potential relevance of certain factors on the resulting directional bias, these are investigated separately in the subsequent sections.

### 5.3.1 Effect of mesh topology

Since the original mesh configuration (Figure 5.7) only offers two main directions (for a given longitudinal cross-section) for the damage band to propagate, whereby none of them is aligned with the observed crack pattern, it is considered appropriate to resort to pentahedrons (wedges), hexahedrons under different orientations or a combination thereof in the vicinity of the notch. By including these mesh topologies, which in turn increase the number of available main directions, it is intended to see if the damage propagation is able to overcome the alignment tendency and reflect more accurately the test crack pattern. Figure 5.11 shows the alternative mesh configurations considered in this regard.

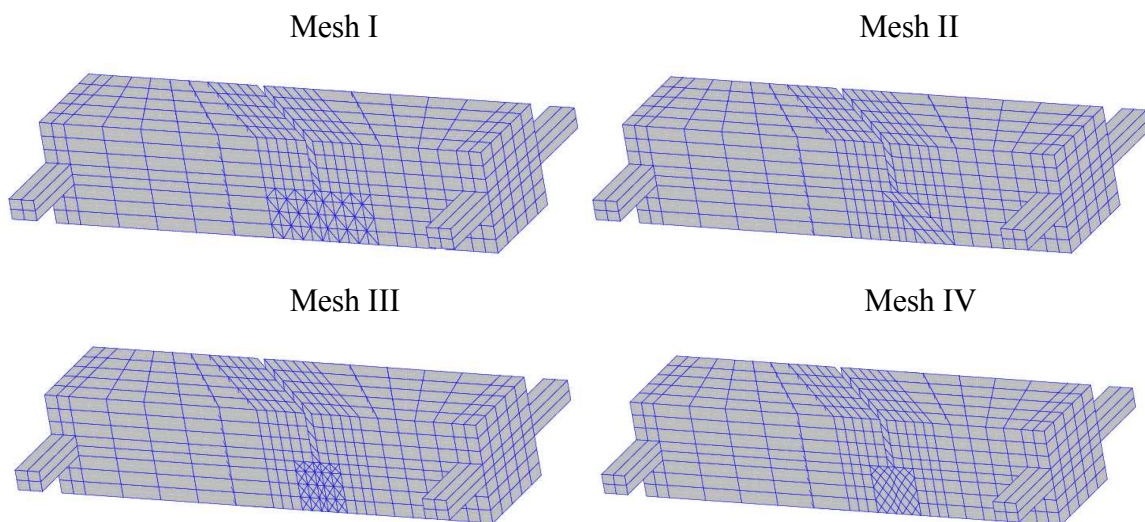


Figure 5.11: Alternative mesh configurations around the notch

Changing the element type and orientation has an immediate effect on the characteristic element size  $h$  when considered as a fixed parameter. Following a similar parametric approach as with the original mesh leads to the improved values of  $h$  shown in Table 5.1. In the absence of test data, a qualitative estimation of  $h$  based on the projection method described in Chapter 3 would serve as initial value, but a sensitivity study on factor  $\gamma$  for highly localised failure modes would be necessary.

| Mesh type | $h$ [mm] |
|-----------|----------|
| I         | 3.5      |
| II        | 5.0      |
| III       | 2.5      |
| IV        | 5.0      |

Table 5.1: Characteristic element size as a function of the mesh type

Interestingly, the distribution of the values listed in Table 5.1 does not only ensue from differences in the element size of each mesh region, but already indicates differences in damage propagation. The response curves in terms of load and CMOD are collected in Figure 5.12. Mesh III, *a priori* the one enabling the greatest number of directional possibilities, is indeed the configuration best reflecting energy dissipation. This feature, however, proves insufficient when assessing the orientations of the propagated damage bands, shown in Figures 5.13-5.16 for advanced states of damage.

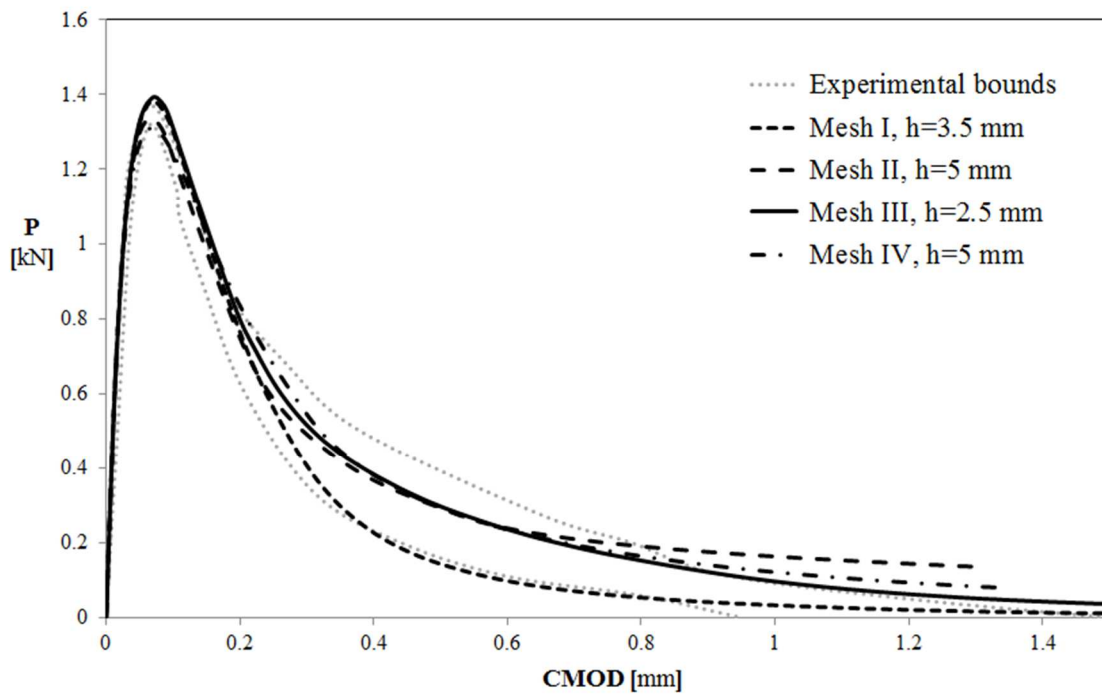
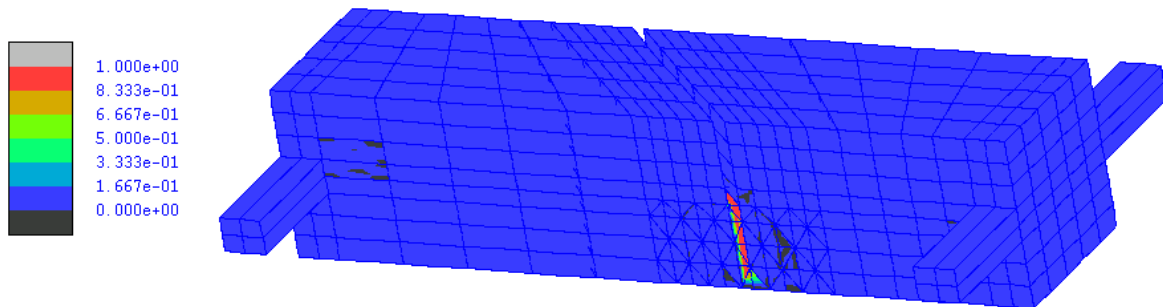
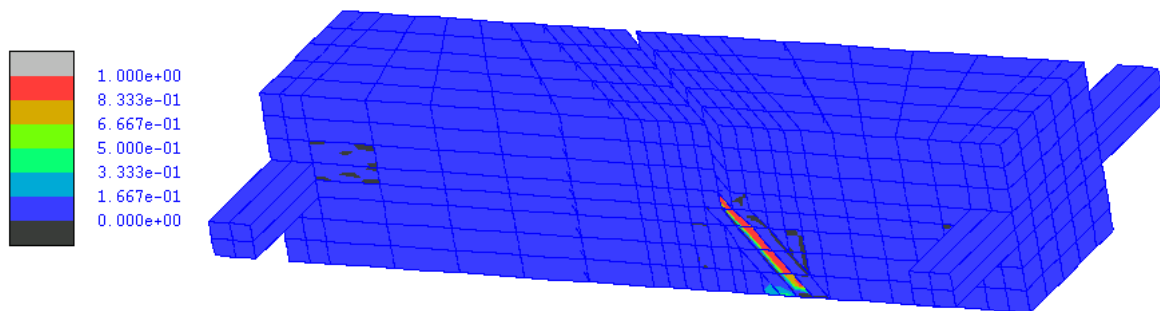
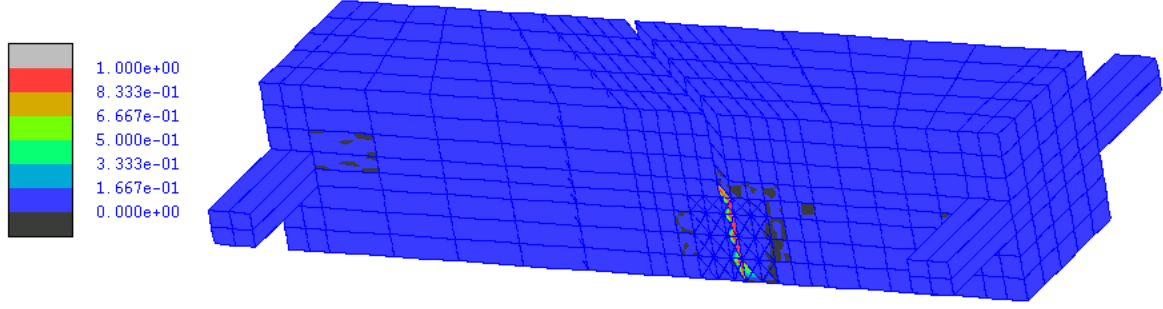
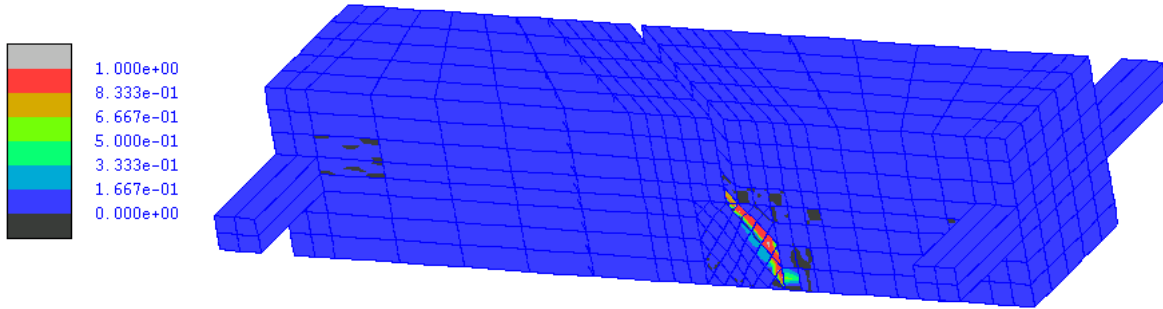


Figure 5.12: Load-CMOD curves for all mesh types

Figure 5.13: Damage variable  $\omega$  distribution for Mesh IFigure 5.14: Damage variable  $\omega$  distribution for Mesh II

Figure 5.15: Damage variable  $\omega$  distribution for Mesh IIIFigure 5.16: Damage variable  $\omega$  distribution for Mesh IV

Mesh I does not involve any noticeable alleviation of directional bias, as the damage band propagates vertically and only manages to slightly warp off the notch plane in the bottom element layer. In Mesh III (Figure 5.15), the damage band propagates in a criss-cross manner but still following the main vertical direction, as the wedges represent a subdivision of the original hexahedrons and the vertical and longitudinal lines show a very strong influence on propagation. Removing the sides aligned with the original mesh in the subdomain surrounding the notch actually transforms Mesh III into Mesh IV. The latter is the only configuration allowing for the damage band to evolve as per the observed experimental crack pattern. To illustrate that the propagation of damage has the right tendency to evolve along the observed directions if the mesh alignment is not too constraining, Figure 5.17 compares the opposite side of the specimen for Meshes II and IV.

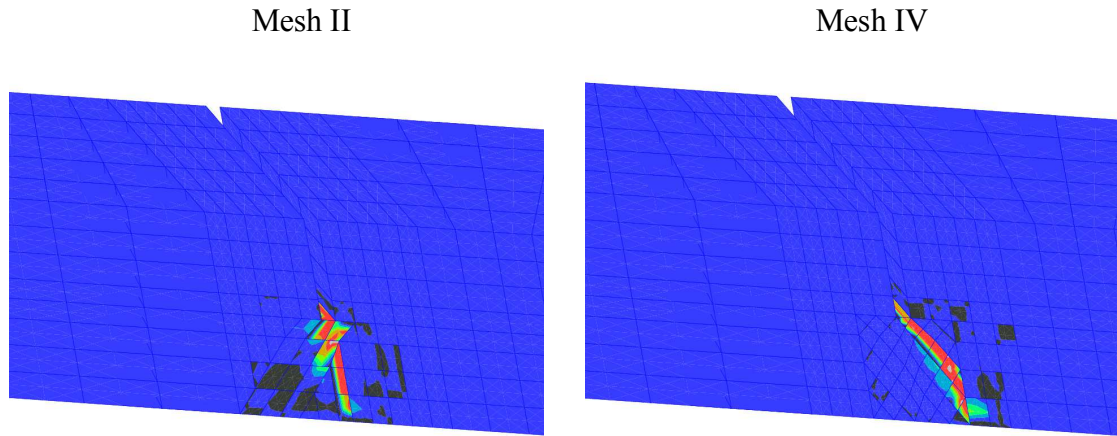


Figure 5.17: Damage variable  $\omega$  distribution in the rear side of the specimen

Whilst Mesh II comprises skewed hexahedral elements identically oriented at both sides of the specimen, Mesh IV arranges the hexahedrons as rhombi, thereby making both diagonal directions available. Figure 5.17 shows clearly that the strong diagonal direction constraint from the skewed hexahedrons in Mesh II is overcome by the damage band, which tends to redirect itself but cannot amend direction further once aligned with the original vertical mesh lines. With the rhombi in Mesh IV, on the contrary, the damage band propagates along the expected diagonals at both sides of the specimen. Figure 5.18 shows one half of Mesh IV under advanced failure for ease of comparison with the experimental crack pattern.

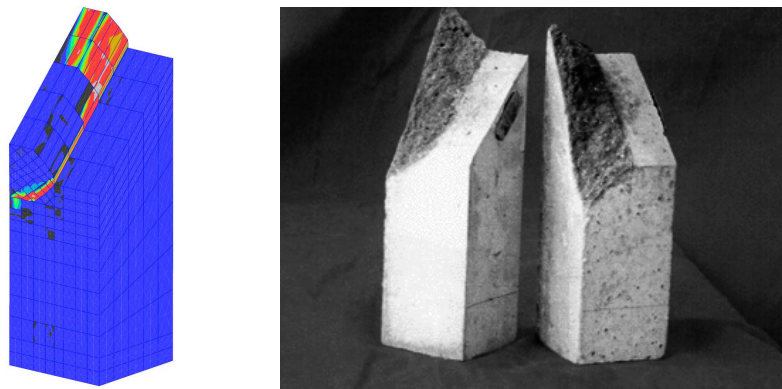


Figure 5.18: Damage distribution after failure with Mesh IV and split specimen blocks  
(Barr and Brokenshire, 1996)

It is noteworthy that, for all alternative Meshes I-IV, the onset of instabilities detected in Section 5.3 and depicted in Figure 5.8 is no longer present. This could be an unexpected consequence of replacing the hexahedrons with a line of wedge elements at the notch tip. If the analysis based on the original mesh (Figure 5.7) is repeated with an artificially enhanced

value of fracture energy  $G_f$ , thereby greatly slowing down damage evolution and accentuating the plastic deformations, the deformed shape around the notch follows the pattern shown in Figure 5.19a, where an amplification factor of 20 is applied.

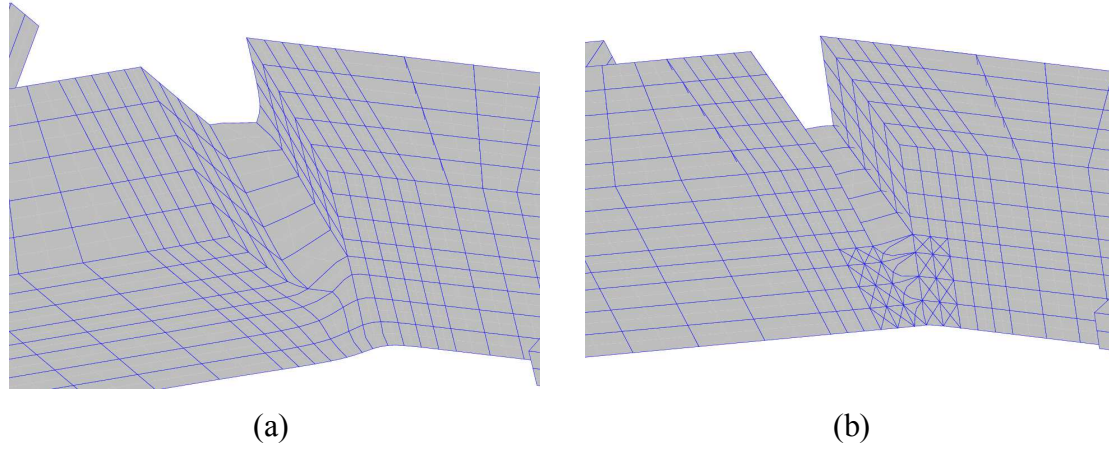


Figure 5.19: Deformed shape after failure (a) Original mesh with artificially high  $G_f$   
(b) Mesh III with standard  $G_f$

The hexahedrons at the notch tip deform in such a way that the (principal) plastic strain propagates in the opposite diagonal to the expected crack pattern, whereas the wedges (Figure 5.19b) facilitate that plastic strains propagate towards the right direction (though still constrained by directional bias). Further insight to check if resorting to anisotropic damage alleviates instability can be found in Section 5.3.3.

### 5.3.2 Effect of localisation analysis

As elaborated in Chapter 3, based on the good directional properties expected from the material model as shown by localisation analysis, it is investigated here if resorting to this tool to redefine the relation between Cartesian and principal directions entails any significant benefit in terms of alleviation of the mesh induced directional bias. Due to the purely local character of localisation analysis, it seems reasonable to expect a directional evaluation with a greater likelihood of mesh orientation independence.

Figure 5.20 shows a comparison in the load-CMOD curve, for the original mesh depicted in Figure 5.7, between the standard simulation and the extended one including localisation analysis. As expected, there are no appreciable changes in the global response; however,

despite such analysis driving the propagation of plastic strains, directional bias is not overcome, and the damage band evolves following the vertical mesh lines, as depicted in Figure 5.21.

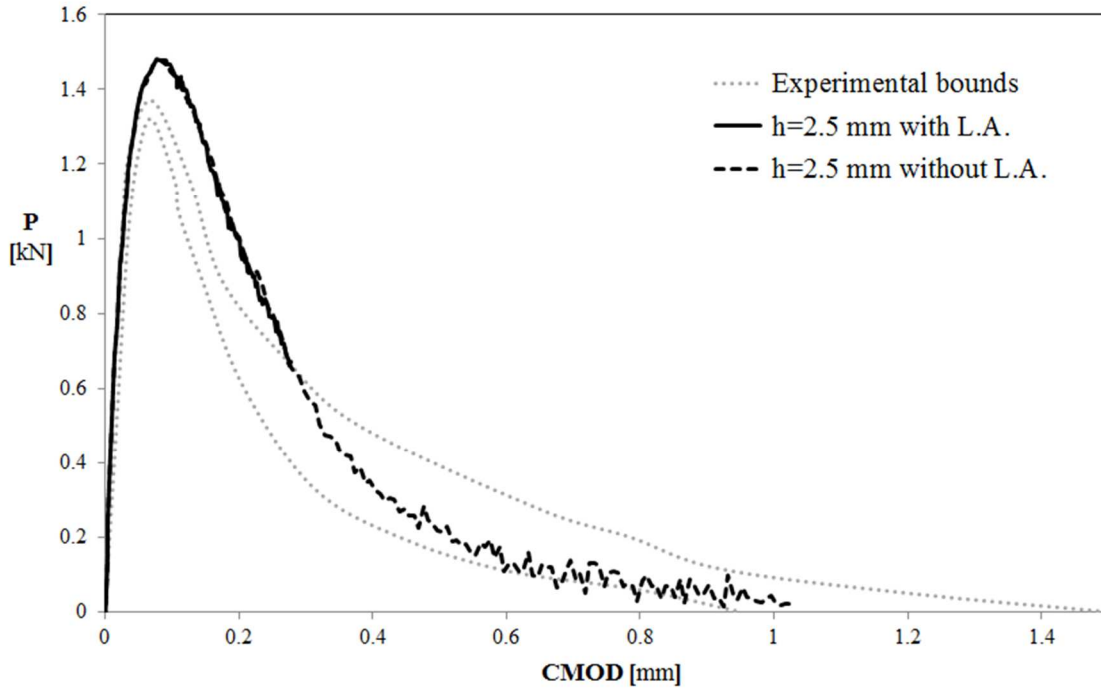


Figure 5.20: Load-CMOD curves with and without resorting to localisation analysis (L.A.)

The onset of instabilities at post-peak cannot be overcome either, and the computational demand is greater when compared to standard analysis, as for every Gauss point the determinant of the localisation tensor must be tracked to detect its potential singularity. The convergence rate is observed to decay, with requirements of higher iteration number or reduction of incremental step size. Consequently, and despite being a promising tool from the mathematical point of view, localisation analysis does not seem to be able to provide additional resources with which to address mesh induced directional bias.

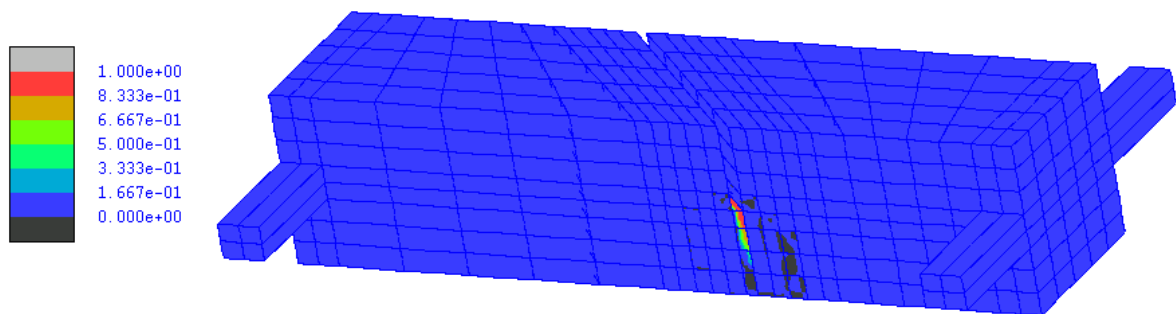


Figure 5.21: Damage variable  $\omega$  distribution with localisation analysis

### 5.3.3 Effect of anisotropic damage

The extension of the CDPM to anisotropic damage, as presented in Chapter 3, is applied here to investigate if such change in the character of the damage law has any effect on the global response or the propagation of the damage band. Figure 5.22 shows the load–CMOD curve resulting from analysis of the original mesh (Figure 5.7) and alternative Mesh IV (Figure 5.11). Peak load is predicted identically to the case of isotropic damage and the post-peak branch is traced adequately, although at a certain level of damage after failure (CMOD value of approximately 0.25 mm) it is computationally more expensive for the iterative procedure to continue, as convergence may not be attained for the same incremental step as with isotropic damage.

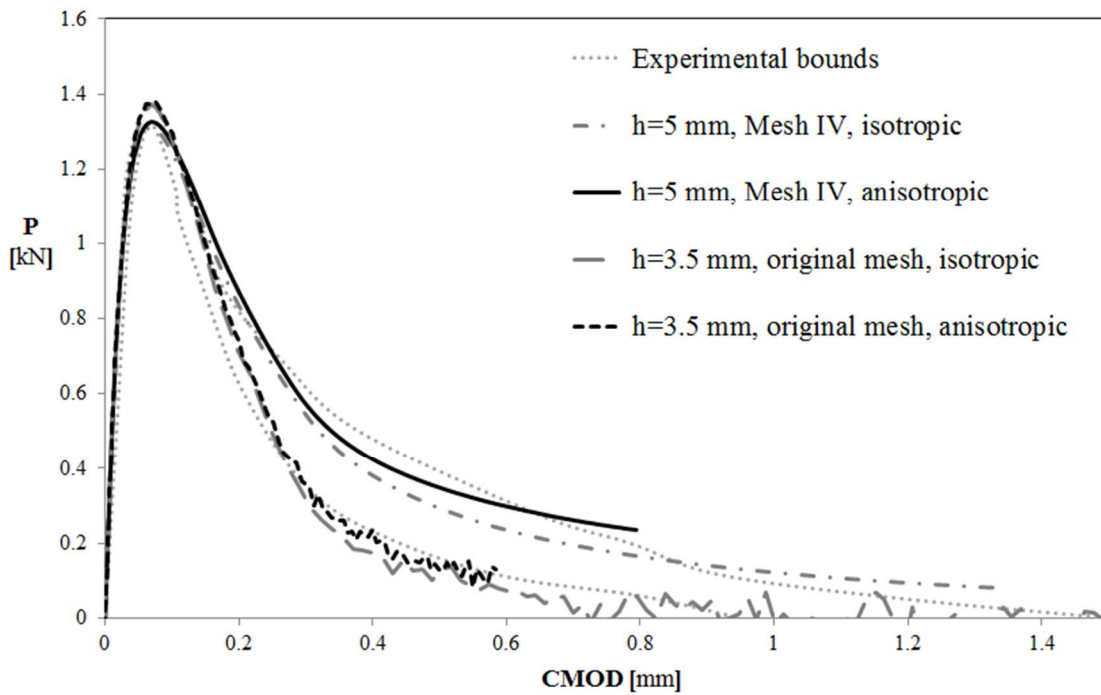


Figure 5.22: Load-CMOD curves resorting to anisotropic damage

In any case, the mesh induced directional bias has the same influence on damage propagation as in Section 5.3.1, as can be seen in Figure 5.23, where the first principal damage component displays the same tendency as the isotropic scalar damage variable to align with the directions of the mesh lines. Further investigation on the application of anisotropic damage can be found in the first major case study of Chapter 7.

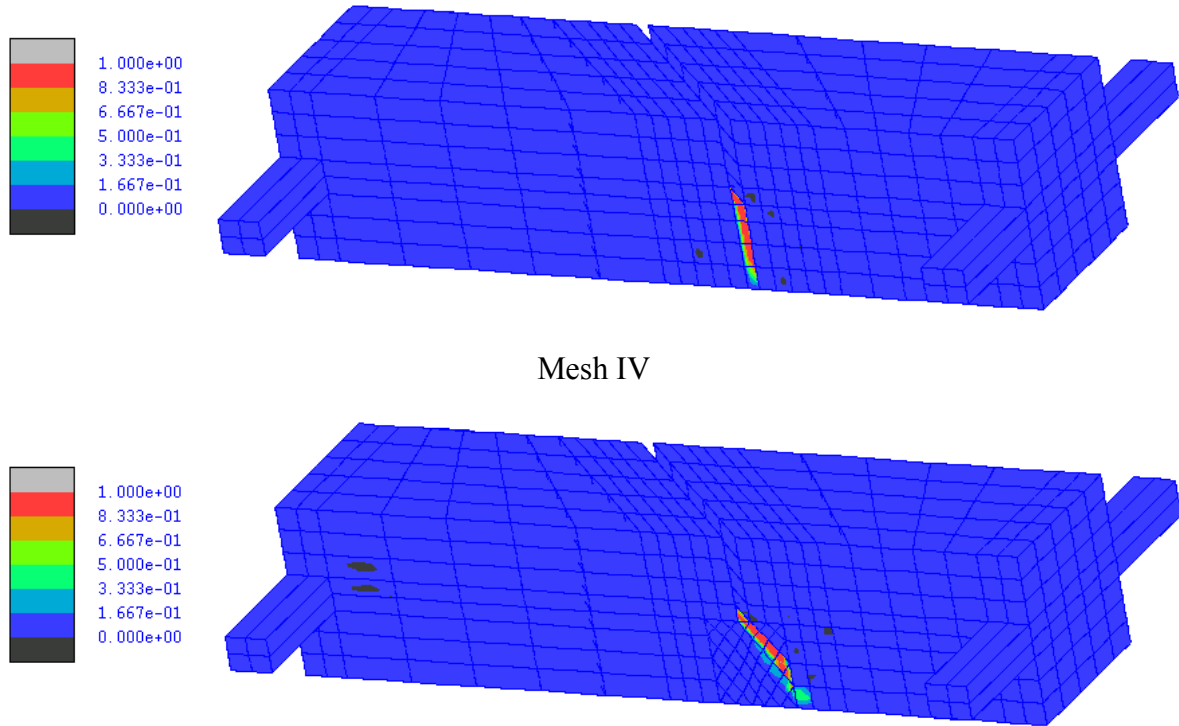


Figure 5.23: Distribution of the first principal value of damage tensor  $\omega$  (CMOD  $\sim 0.6$  mm)

## 5.4 Torsion-bending beam

This test pertains to a series of two- and three-dimensional stress state experiments carried out in the University of Innsbruck (Feist, 2004). Specifically, the series called PCT-3D (plain concrete test) focuses on corner notched beams of square cross-section subject to an eccentric vertical load applied through a rigid steel roller, whereby the eccentricity of the load gives rise to a combined bending and torsional effect. Consequently, the character of the test, as well as the spatial evolution of the damage surface, is fully three-dimensional.

The beam geometry and setup are schematically shown in Figure 5.24. A thorough description of the experimental layout can be found in Feist (2004).

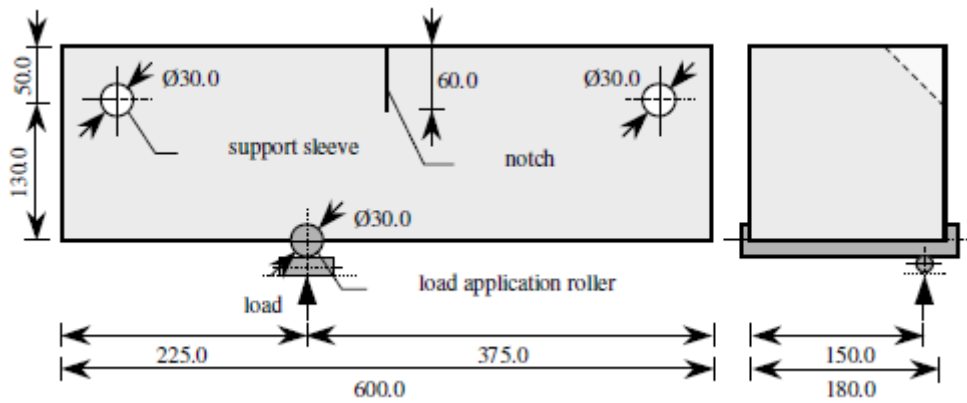


Figure 5.24: Dimensions (in mm) and experimental layout of PCT-3D  
(Feist and Hofstetter, 2004)

Initially, and based on Valentini and Hofstetter (2013), a structured mesh of 65304 20-noded hexahedral elements with reduced Gauss integration is used to discretise both the concrete beam and the steel rollers for support and load application, as depicted in Figure 5.25. Also, following the same reference, appropriate boundary conditions are enforced along the outermost seven nodes of each roller axis, and the load is applied for static analysis under vertical displacement control of the node offset 60 mm from the longitudinal vertical midplane, in the direction of the notch. At a certain stage, this node displacement control is replaced by an arc-length control strategy.

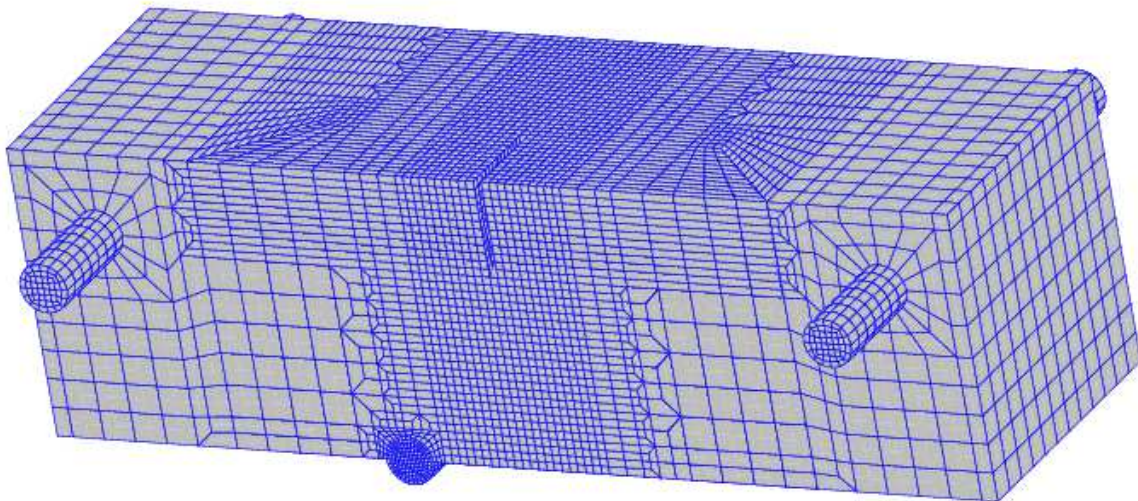


Figure 5.25: Mesh for the simulation of PCT-3D consisting exclusively of isoparametric 20-noded hexahedral elements

The material parameters are taken originally from Feist (2004), with due consideration to the remarks in Valentini and Hofstetter (2013) regarding the tensile strength and the fracture energy, as follows:

$$E_c = 37292.60 \text{ MPa}$$

$$\nu_c = 0.1927$$

$$\bar{f}_c = 40.12 \text{ MPa}$$

$$\bar{f}_t = 3.05 \text{ MPa}$$

$$G_f = 66.10 \text{ J/m}^2$$

$$E_s = 210000.00 \text{ MPa}$$

$$\nu_s = 0.30$$

The characteristic element size is conservatively taken as  $h = 2.5 \text{ mm}$ , i.e. half of the size of elements across the notch width. Figure 5.26 shows the resulting curve from static analysis, displaying the vertical load  $\mathbf{P}$  in terms of the crack-mouth-opening-displacement (CMOD), along with the experimental scatter. The CMOD is measured across the notch, between the two corner nodes.

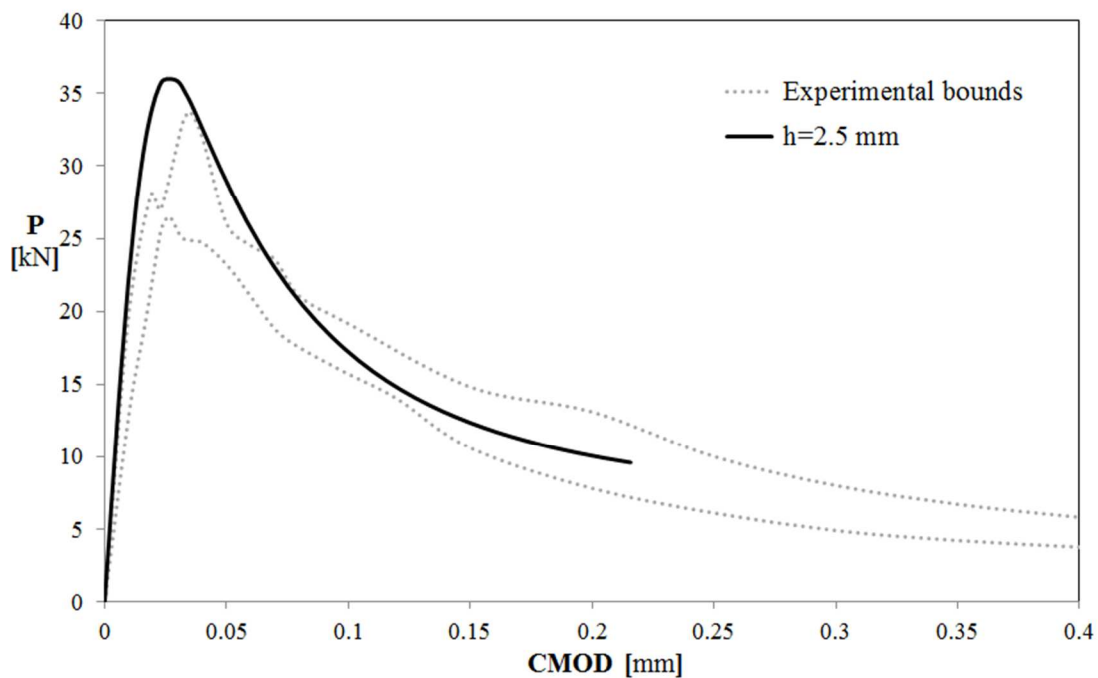


Figure 5.26: Load-CMOD curve and experimental scatter for PCT-3D

The peak load of the simulation ( $P_{\max} \approx 36 \text{ kN}$ ) overestimates the average recorded load (averaging the measurements of four specimens within the bounds of Figure 5.26) by

approximately 28%, although the associated CMOD value (0.024 mm) corresponds very well with the experimental measurement. Moreover, the softening branch of the curve is tracked steadily and shows a progressively better correspondence with the test scatter with increasing CMOD. In light of the resulting damage band, a larger value of the characteristic element size  $h$  would have been more suitable, which in turn would have reduced the predicted peak load.

It is worth noting that the arc-length strategy allowed for equilibrium tracing past a point of snap-back considering the vertical displacement under the load, as shown in Figure 5.27. It is not possible to contrast this feature with the recordings of the inductive displacement transducers used in the tests since, according to Feist (2004), the values obtained with these devices are not reliable due to local nonlinearities around the point of load application.

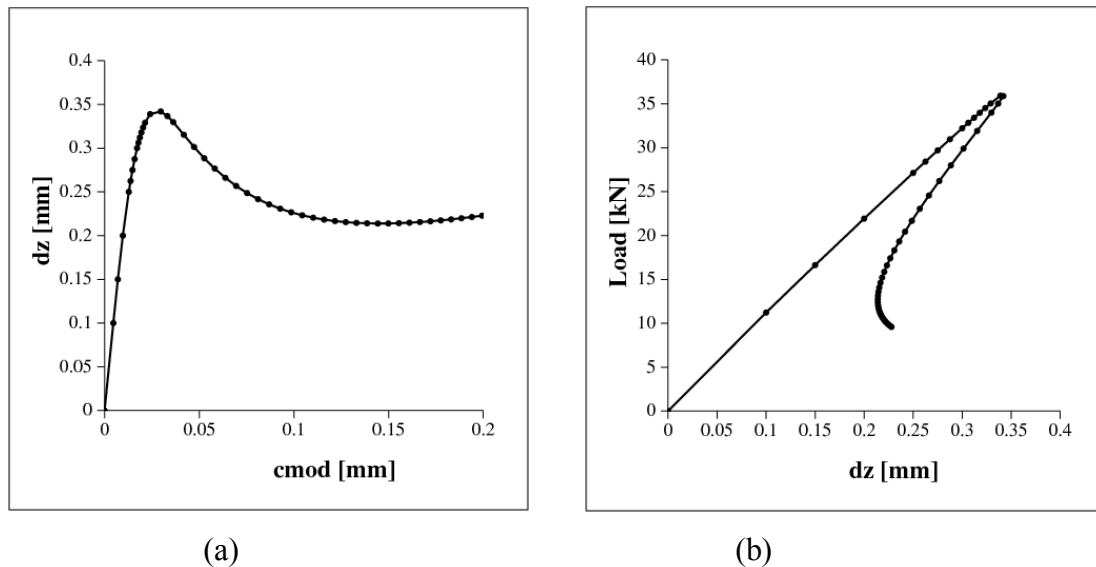


Figure 5.27: (a) Vertical displacement vs. CMOD (b) Load vs. vertical displacement

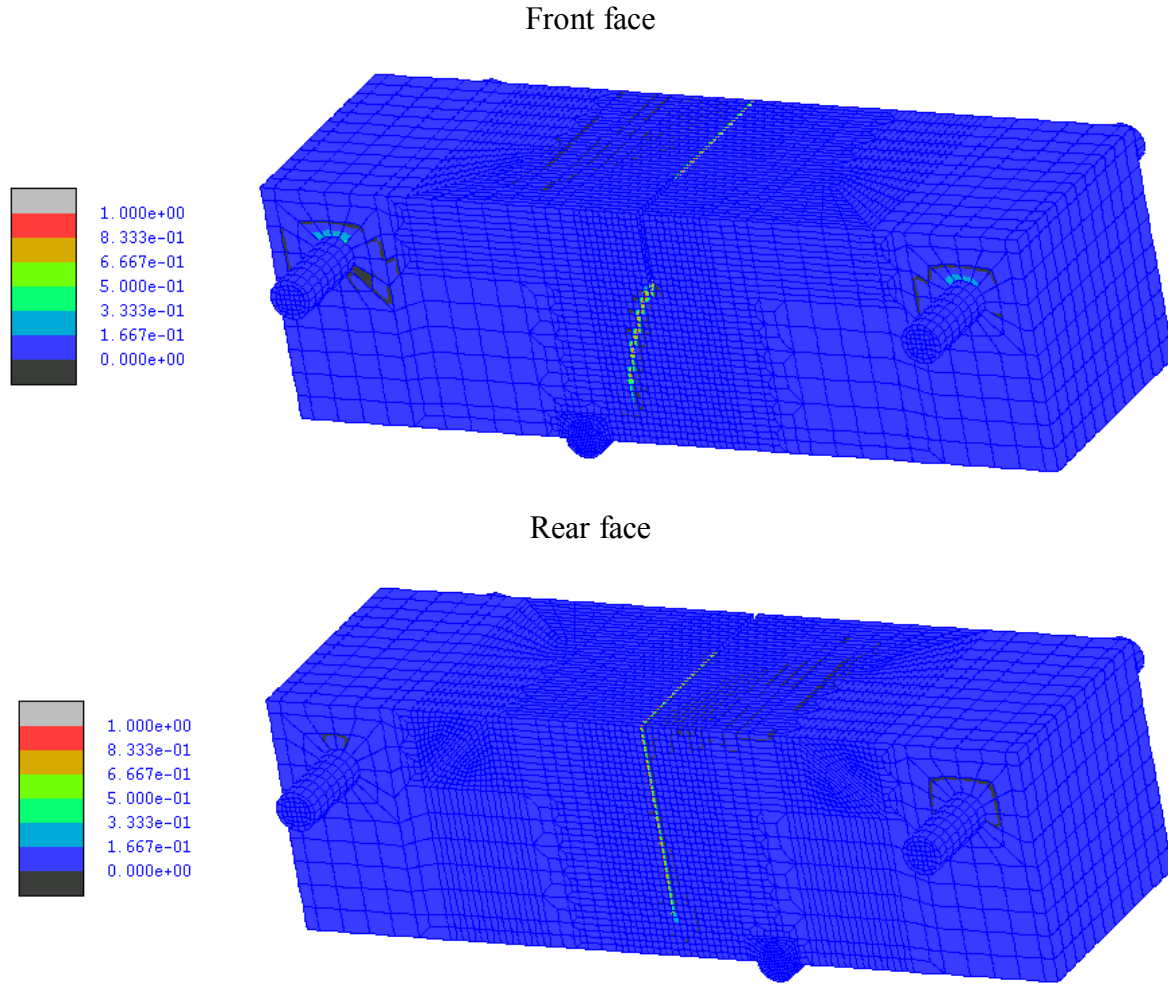


Figure 5.28: Distribution of  $\omega$  at post-peak (CMOD  $\sim 0.024$  mm)

The scalar damage variable  $\omega$  distribution at post-peak is depicted in Figure 5.28. As commented by Gasser (2007) and reported by Feist (2004), the observed crack pattern is curved on all four faces of the specimen, whereas the predicted evolution of damage has a strong tendency to align with the mesh orientation in the top and rear faces. Hence, the mesh-induced directional bias anticipated in Chapter 3 and discussed in Section 5.3 is affecting the spatial output of the simulation. It remains interesting to investigate whether the re-meshing of the top face, enabling more orientation alternatives for damage propagation, alleviates directional bias, though it is not pursued further here.

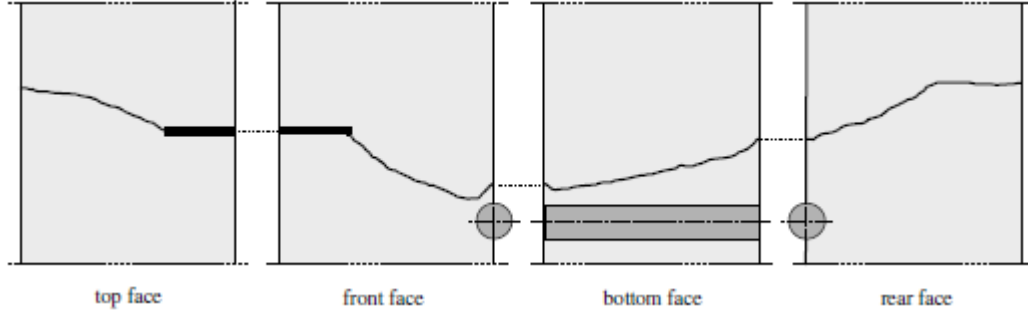


Figure 5.29: PCT-3D averaged observed crack pattern (Feist and Hofstetter, 2004)

In order to further compare the experimental crack pattern (for reference included in Figure 5.29) with the predicted damage distribution, focus is shifted from static to dynamic analysis, specifically of the explicit type with a Hilber-Hughes-Taylor (HHT) integration scheme. Integration parameters  $\alpha$ ,  $\beta$  and  $\gamma$  are chosen as:

$$\alpha = -\frac{1}{3}$$

$$\beta = \frac{(1-\alpha)^2}{4}$$

$$\gamma = \frac{1-2\alpha}{2}$$

A linear impulsive curve is defined in order to induce a vertical displacement of constant velocity in the same node where the load is applied. Resorting to hierarchical partition modelling (Jokhio, 2012; Jokhio and Izzuddin, 2015) with 5 partitions (with an element ratio of approximately 1.8 between the largest and the smallest partition) leads to the damage distribution shown in Figure 5.30.

The directional bias is not noticeably alleviated. However, the three-dimensional character of the localisation (damage) band is captured well. Illustratively, this can be seen in Figure 5.31, where the spatial surface of the fully damaged material is cut by the cross-sectional plane containing the notch edge furthest away from the load application roller (Figure 5.28a). The resulting contour corresponds adequately with the 0-isoline of the observed crack surface in Figure 5.31b.

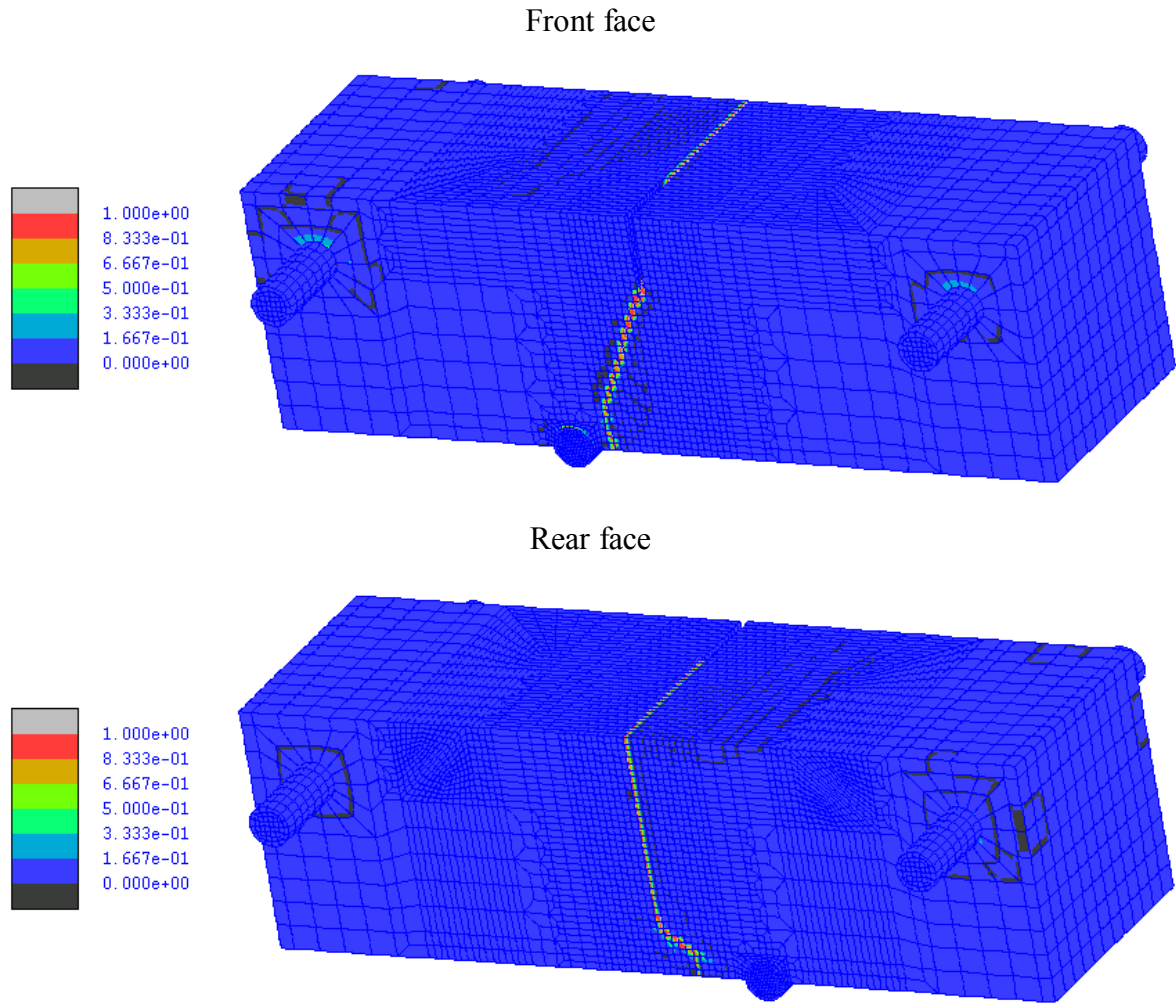


Figure 5.30: Distribution of  $\omega$  at post-peak (CMOD > 1 mm), under explicit dynamic analysis

Furthermore, the predicted damage spatial distribution along the four faces of the specimen is shown in Figure 5.32, where a good correspondence with the experimental crack pattern of Figure 5.29 is noted particularly in the front and bottom faces, not (or less) affected by the directional bias.

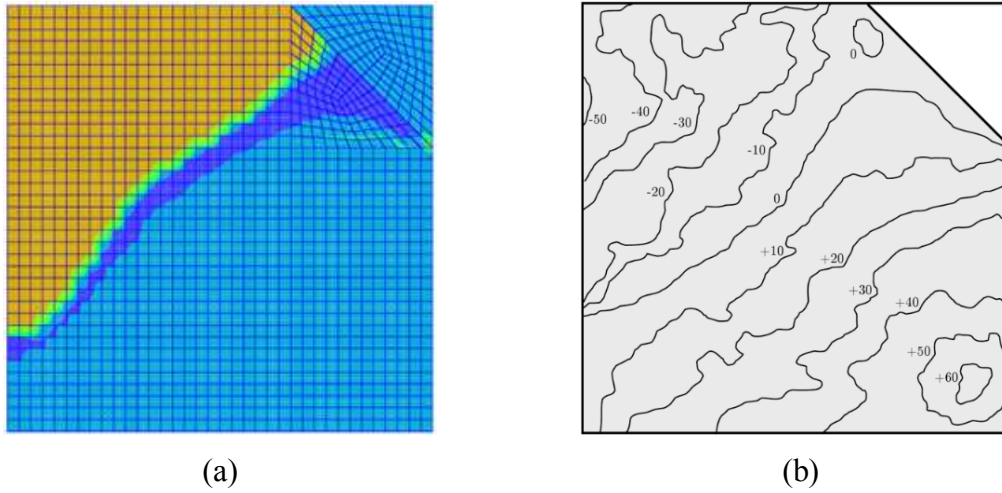


Figure 5.31: (a) Distribution of  $\omega$  along the cross-section containing a notch edge (CMOD > 1 mm, under dynamic analysis) (b) Isoline representation of the crack surface for a PCT-3D specimen along the midspan cross-section (Feist, 2004)

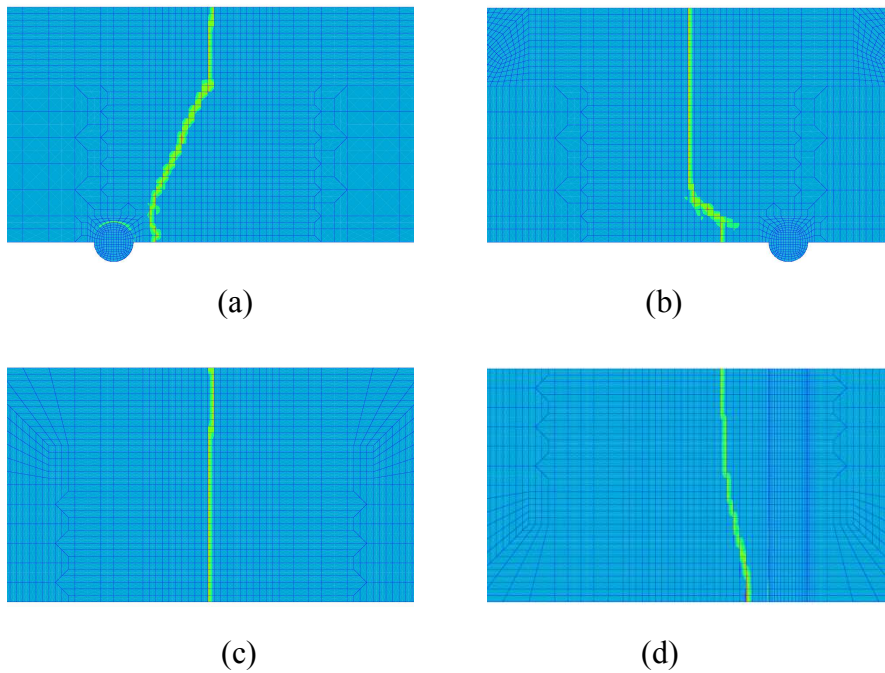


Figure 5.32: Predicted damage distribution along all faces of the PCT-3D dynamic simulation: (a) front face (b) rear face (c) top face (d) bottom face

Additionally, the arisen benefits of partitioned modelling are significant, as the explicit dynamic analysis manages to increase the number of outputs by an approximate factor of 6.4 compared to static analysis, for the same computing time.

The response curve under dynamic analysis (see Figure 5.33) indicates that the peak load can be estimated in a qualitatively similar manner to static analysis, although the post-peak branch is sensitive to dynamic effects. These are considered as potentially removable by resorting to a different (spatial) discretisation of the steel rollers, in particular the load application one. A coarser discretisation would reduce the maximum natural frequency of the beam, allowing a larger time-step to be used, thus facilitating a slower application of loading which should reduce dynamic effects under displacement control conditions.

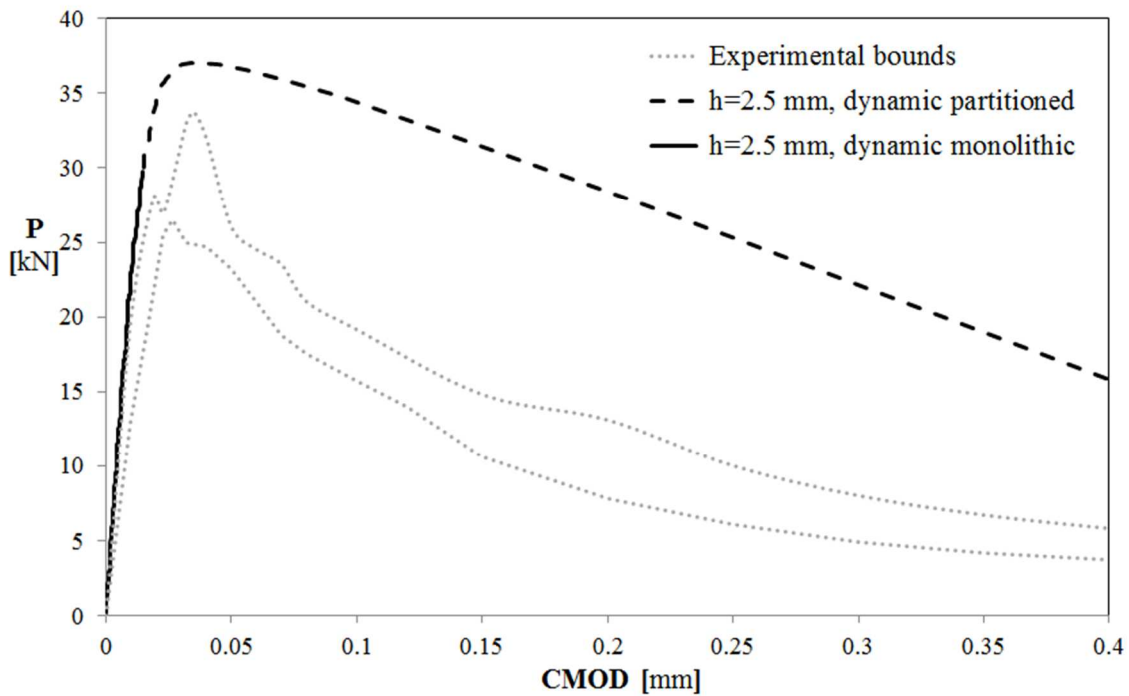


Figure 5.33: Load-CMOD curve and experimental scatter for PCT-3D, under explicit dynamic analysis, *monolithic* and partitioned

As a further confirmation of the computational benefit of partitioning, Figure 5.33 includes the response curve of a *monolithic* model (i.e. without partitioning) under dynamic analysis with identical parameters. In such case, the same computational resource is insufficient to trace the response up to and beyond the peak load.

In light of all results for this simulation, static analysis is preferred in this case, as it provides an accurate load-CMOD response whilst still displaying a reasonable crack pattern.

## 5.5 Uniaxial compression

In the numerical examples presented hitherto, the predominant stress states guiding damage are tensile. This section aims at illustrating the activation and propagation of damage under compressive states, in particular under uniaxial conditions. To this end, the standard compression tests of cube and cylinder specimens are simulated. It is worth noting that the characteristic element size  $h$  maintains its character of fixed parameter, notionally estimating the damage bandwidth in the spirit of a projection method, as is the case for all previous tensile examples.

### 5.5.1 Cube test

A prismatic cube specimen of the conventional dimensions for compressive testing (150 mm size) is modelled with 216 isoparametric hexahedrons (Figure 5.34).

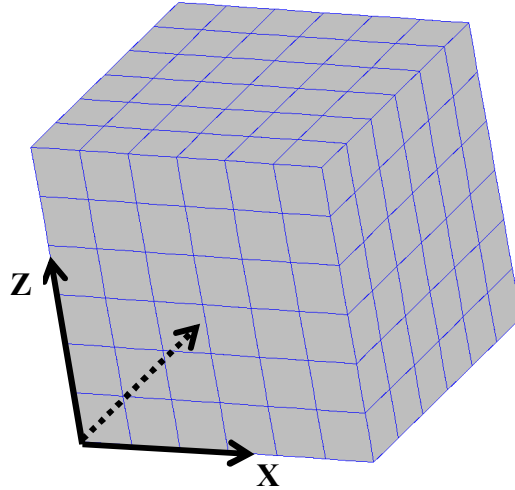


Figure 5.34: Mesh for the cube compression test

The set of material parameters is illustratively taken as the following:

$$E_c = 19305 \text{ MPa}$$

$$\nu_c = 0.20$$

$$\bar{f}_c = 22.10 \text{ MPa}$$

$$\bar{f}_t = 2.76 \text{ MPa}$$

$$G_f = 100 \text{ J/m}^2$$

The characteristic element size is assumed as  $h = 18 \text{ mm}$ . Both the top and bottom faces of the cube have prescribed displacements in the  $Z$  direction, with the base being restrained and the top having a uniform downward displacement controlling the analysis throughout. The lateral restraint at these faces, reflecting the confining effect of the test platens, is set at its extreme values (full fixity and free lateral expansion) to ensure that the resulting bounds

embed the intermediate response that would best reflect the platen effect. In order to facilitate the onset of localisation, an imperfection in the form of a 10 % reduction of the compressive strength of a central element is introduced.

Figure 5.35 shows the curves of the vertical force resultant  $R$  vs. the downward displacement  $w$  of the top face, for both platen restraining assumptions. As expected, upon reaching of the compressive strength, the response undergoes softening as a result of damage propagation. The peak load values correspond to the nominal mean stresses shown in Table 5.2.

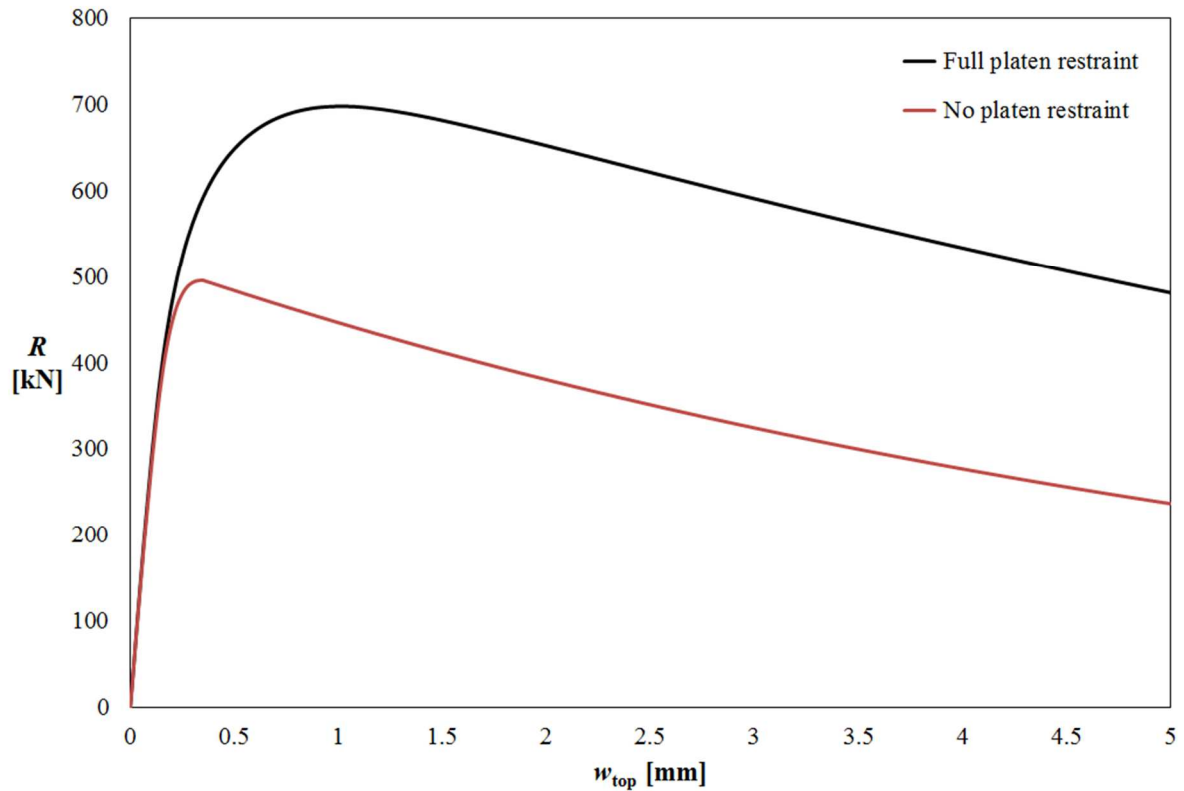


Figure 5.35: Response curves of cube compression test for different lateral restraints

|                          | Full restraint | No restraint |
|--------------------------|----------------|--------------|
| $R_{\max}$<br>[kN]       | 697.8          | 495.4        |
| $\sigma_{\max}$<br>[MPa] | 31.0           | 22.0         |

Table 5.2: Maximum values of load and nominal mean stress

From Table 5.2 and the initial set of material parameters, it can be concluded that  $\bar{f}_c$  reflects the cylinder strength, leading to a platen effect between the extreme bounds for any reasonable cylinder to cube strength ratio, as shown in the next section. Illustratively, Figure 5.36 depicts the distribution of the scalar damage variable at post-peak for the case of full platen restraint:

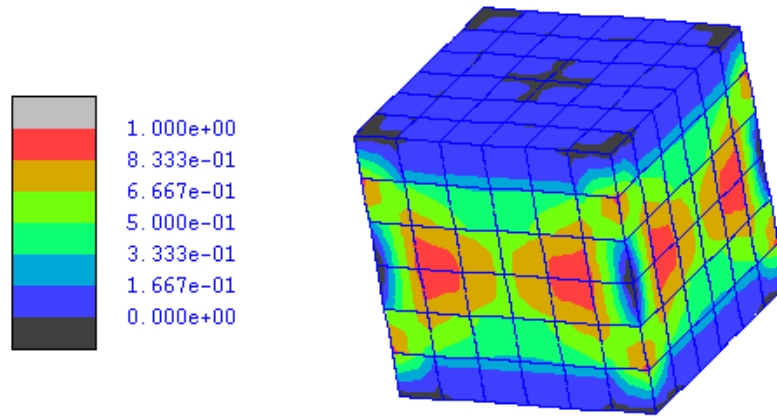


Figure 5.36: Scalar damage distribution of the cube test for  $w_{top} = 5$  mm

Despite the overestimation of strength under fully confined conditions, the directional features of the resulting damage bands are in reasonable good agreement with observed crack patterns, as anticipated in the notional single element compression test of Chapter 3.

### 5.5.2 Cylinder test

The standard cylinder for the compression test, of 150 mm diameter and 300 mm height, is modelled with 576 isoparametric hexahedrons, as shown in Figure 5.37.

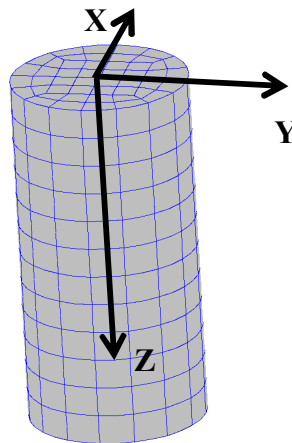


Figure 5.37: Mesh for the cylinder compression test

The set of material parameters coincides with the adopted one for the cube test in the preceding section. The characteristic element size also maintained as  $h=18$  mm. A 10% weakening of compression strength in a central element is also assumed. For simplicity, only full lateral platen restraint configuration is considered in the vertical displacement controlled analysis. The resulting force vs. top displacement curve is shown in Figure 5.38.

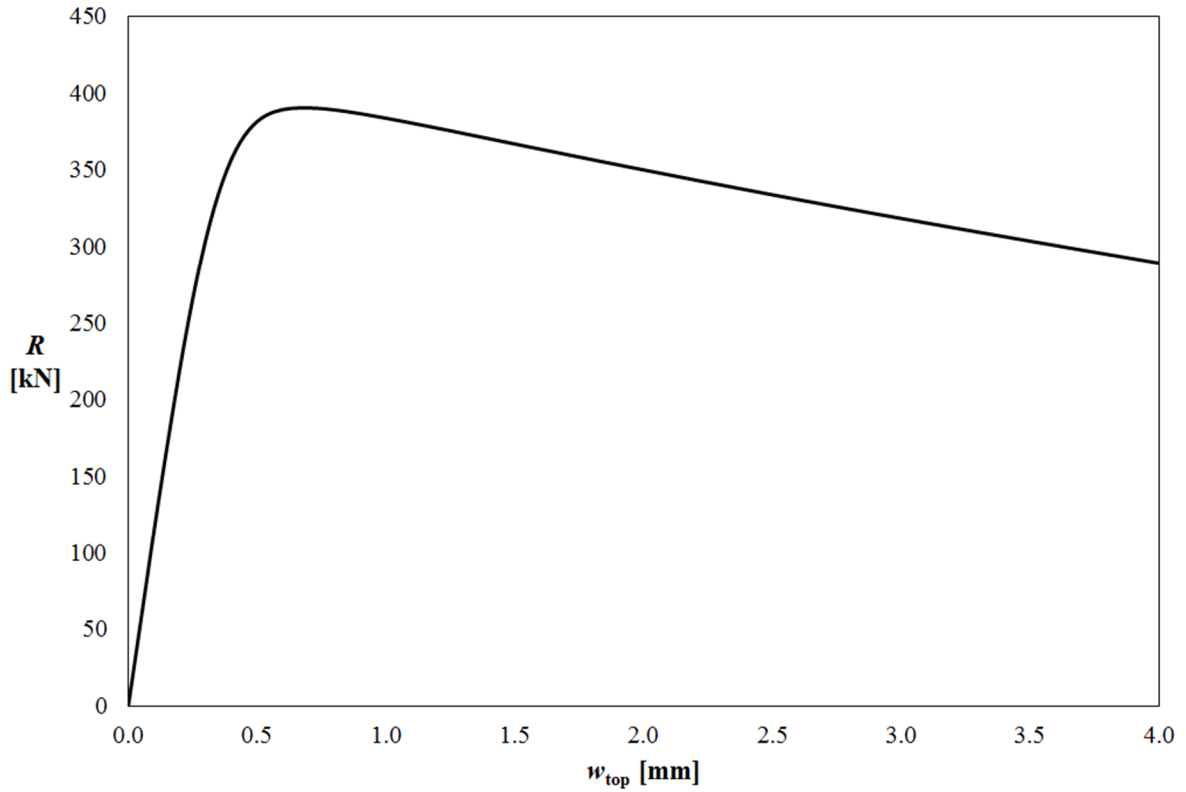


Figure 5.38: Response curves of cylinder compression test for full lateral platen restraint

The peak load value is  $R_{max} = 390.5$  kN, which in turn implies a maximum nominal mean stress  $\sigma_{max} = 22.1$  MPa. Consequently, the ratio of maximum mean stress values for cylinder and cube tests is approximately 0.71. As comparative reference, the ratio considered in EC2 for strength values ranging between 12 MPa and 90 MPa oscillates around 0.80, with a minimum of 0.78 and maximum of 0.86.

The scalar damage distribution at post-peak is depicted in Figure 5.39. Although damage propagates from the middle third of the specimen, where uniaxial conditions are best reflected, and despite the accurate local evaluation of damage orientation illustrated by localisation analysis in Chapter 3, the damage propagation follows the main mesh direction.

Hence, compressive states give rise to solution fields affected by mesh induced directional bias to the same extent as tensile states.

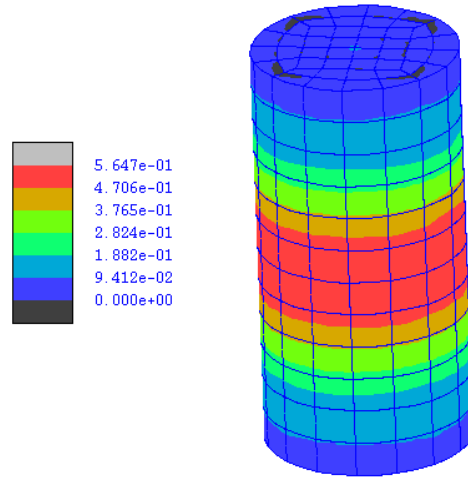


Figure 5.39: Scalar damage distribution of the cylinder test for  $w_{top} = 4$  mm

## 5.6 Reinforced concrete beam loaded at midspan

This numerical example deals with the simulation of the structural response of two specimens originally tested by Karihaloo (1992), with the experimental setup and geometry as shown in Figure 5.40. The concrete bulk dimensions coincide in both beams, having a rectangular cross-section with a depth of 150 mm and a width of 100 mm, along with a span length of 1.6 m between supports. A knife-edge load is applied at midspan through a loading plate. There are no transverse shear links, only longitudinal reinforcement in the tension side of the beam induced by sagging, with the following arrangements:

Beam 1: 1 $\Phi$ 12,  $\rho_s = 0.75\%$

Beam 2: 2 $\Phi$ 12,  $\rho_s = 1.50\%$

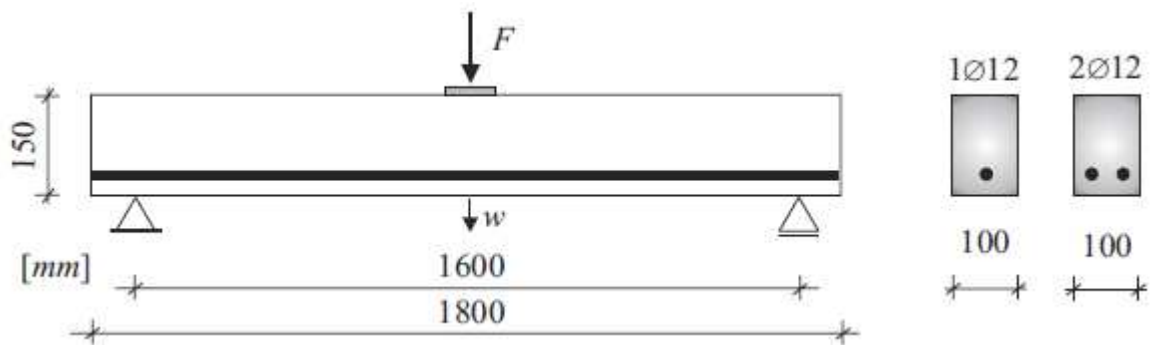


Figure 5.40: Test specimen by Karihaloo (1992): experimental setup, boundary conditions and dimensions (Schütt, 2005)

Although these tests are frequently resorted to in the literature due to their ease of discretisation, there is a striking scatter in the adopted values for the necessary material properties. This is already noted by Schütt (2005), who mostly complies with the values reported by Karihaloo (1992), albeit with an increase in the compressive strength. In the original test report, Karihaloo (1992) states that fracture mix properties were not measured but estimated, and hence the original fracture energy value  $G_f = 50 \text{ J/m}^2$  is a derived magnitude from an estimation of fracture toughness  $K_{Ic}$ . Moreover, Menrath (1999) performed a parametric study of beam 1 with  $G_f$  as free parameter, arguing that the minimum value to be considered, based on CEB-FIP Model Code (1990) estimation guidelines, should be  $G_f = 120 \text{ J/m}^2$ , which is already more than twice the value estimated by Karihaloo (1992). The upper bound for  $G_f$  as per the same guidelines is  $G_f = 200 \text{ J/m}^2$ , which is adopted by Huber (2006), but the parametric study shows that an infinite fracture energy (that effectively corresponds to concrete behaving as ‘perfectly plastic’, since damage cannot progress) leads to the best fit for peak and post-peak behaviour. The greatest finite value considered by Menrath (1999) is  $G_f = 500 \text{ J/m}^2$ , and it maintains the features of lower value curves at post-peak, as well as a reasonable agreement with the curve of Suanno (1995) up to peak. The latter also resorts to plasticity (‘Cap model’) alongside scalar damage, and his predicted pre-peak response shows the best match with the test results. However, the required amount of parameters for the Cap model (9 aside of elastic constants and strength values) together with the scarcity of original reported measurements indicates that calibration based on test results is needed. The plastic hardening modulus, with no original report mention, ranges from  $H = 0 \text{ MPa}$  in Menrath (1999) to  $H = 1.30 \text{ MPa}$  in Schütt (2005), who in turn based this choice on the meso-scale model of Tikhomirov and Stein (2001).

Based on all the above, the set of material parameters adopted for the analysis presented here is the following:

$$\text{concrete} \left\{ \begin{array}{l} E = 30000 \text{ MPa} \\ \nu = 0.2 \\ f_c = 46.0 \text{ MPa} \\ f_t = 3.4 \text{ MPa} \\ G_f = 500 \text{ J/m}^2 \end{array} \right. \quad \text{steel} \left\{ \begin{array}{l} E_s = 200000 \text{ MPa} \\ f_y = 463 \text{ MPa} \\ H = 1.30 \text{ MPa} \end{array} \right.$$

The adopted value for the fixed characteristic element size is  $h = 12.5 \text{ mm}$ . The whole specimen is modelled with 1728 hexahedral elements (Figure 5.41), although the multiple symmetries would allow for reducing it to a subset thereof, accounting in beam 1 for the splitting of the reinforcement bar. To capture the effect of the spreading through the loading plate, the applied knife-edge load is distributed across the plate area.

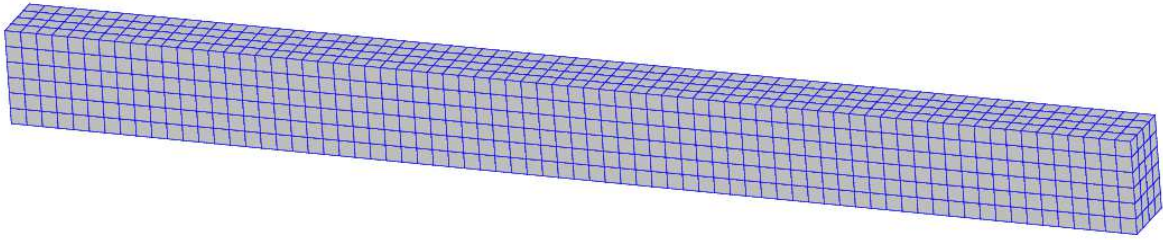


Figure 5.41: Hexahedral mesh for Beams 1 and 2

Figure 5.42 shows the load-displacement response curve resulting from an arc-length strategy based analysis for beam 1, together with the test curve and a scatter comprising the numerical results from simulations by Suanno (1995), Huber (2006), Schütt (2005) and Menrath (1999). The latter three are based on multi-surface plasticity, whereby Huber also includes a gradient-enhanced damage model.

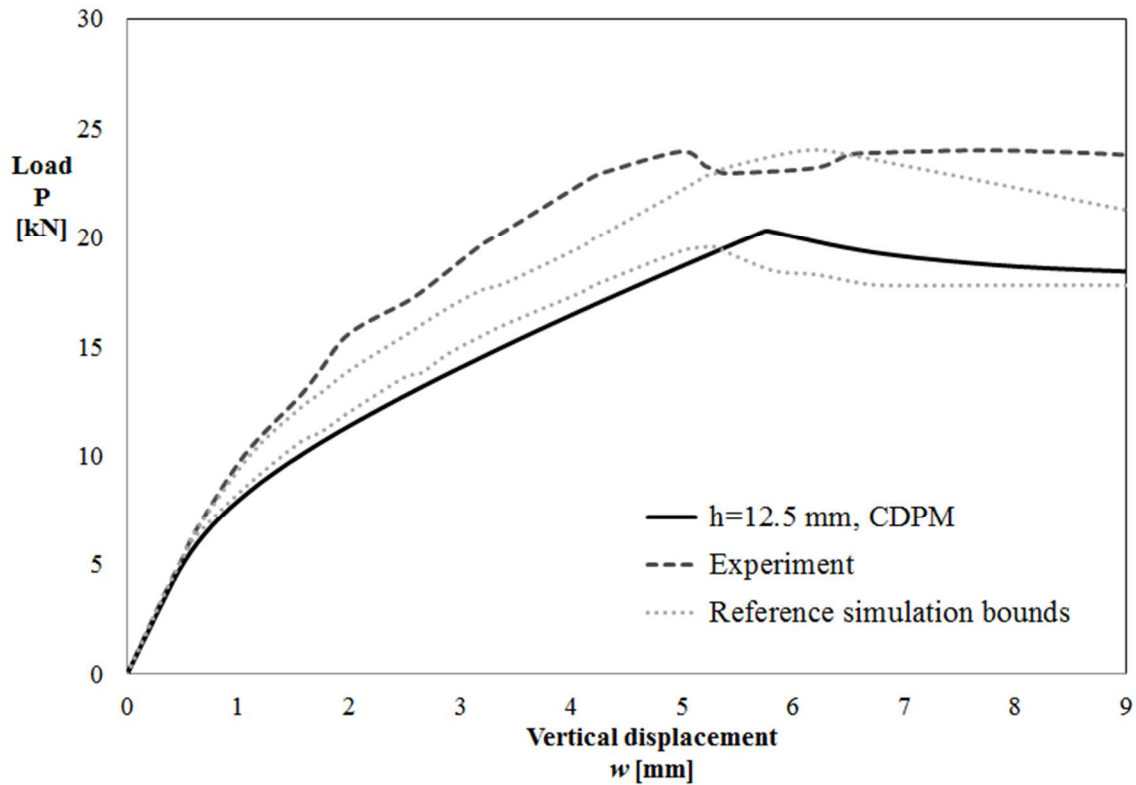


Figure 5.42: Response curve for Beam 1, along with the experimental results and the scatter of numerical results by Suanno (1995), Huber (2006), Schütt (2005) and Menrath (1999)

In Schütt (1995) it is mentioned that collapse of Beam 1 follows from the plastic yielding of the reinforcement bar, which is not in accordance with the reported description of failure. In the original report, Karihaloo (1992) describes the test as a progressive development of flexural cracks until a final diagonal shear crack connecting a pre-existent flexural crack near the support and the loading plate edge is formed. Widening of this shear crack and crushing of the compressive concrete head simultaneously lead to the collapse of the beam.

The current analysis, however, aligns with Schütt's observations, as the peak load is achieved after yielding of the embedded bar. This maximum value  $P = 20.3$  kN corresponds to a vertical displacement of  $w = 5.8$  mm. Although the latter is predicted reasonably (the experimental curve shows a minor decay after peak load before recovering to a higher value at collapse, which remains unexplained and hinders the allocation of a displacement value at peak), the former entails an underestimation of about 15%. With the exception of Menrath (1999), all other reported load predictions achieve a higher peak value. Interestingly, Suanno (1995) (whose curve determines the peak of the scatter in Figure 5.42 and hence achieves the

greatest accuracy) points out that the results of modelling with 8-noded hexahedrons may incur locking effects. To illustrate this potential influence, his analysis is repeated for quadratic 20-noded hexahedrons with 15 integration points, under the same material parameters (calibrated from the 8-noded element based analysis). The predicted peak load then drops to  $P \approx 18.0$  kN, which requires recalibration. As commented by Schütt (2005), and originally Karihaloo (1992), the dowel effect of the reinforcement bar might not have a negligible relevance in the displayed stiffness of the beam, particularly at initial inelastic stages where the plastic (cracking) strains are small to moderate. It is reported by these authors as potentially being the main cause behind the shift between the test and the numerical curves, in the displacement range between the onset of inelastic behaviour and peak load. The influence of dowel action, however, does decrease as cracks develop fully and effectively vanishes upon bar yielding. Hence, it remains unclear if an effect of different nature, like the tension stiffening of concrete between cracks, is more relevant in this regard.

The test curve indicates a nearly perfect plastic post-peak behaviour, whereas all numerical responses display a softening branch. The current model does show a similar behaviour near collapse, which is in line with the parametric study of Menrath (1999). Only unrealistically high values of the fracture energy could accommodate the simulation to the test curve at post-peak, as depicted in Figure 5.43, which suggests that this behaviour relies on a different parameter. On the other hand, artificially high values of fracture energy entail tensile stresses at the cracks not reducing to zero, even after bar yielding, which in turn lead to a progressive overestimation of the flexural capacity as compared to conventional section analysis. As reference, section analysis as per the guidelines of Eurocode 2 (2004) results in a strength value of approximately 16 kN.

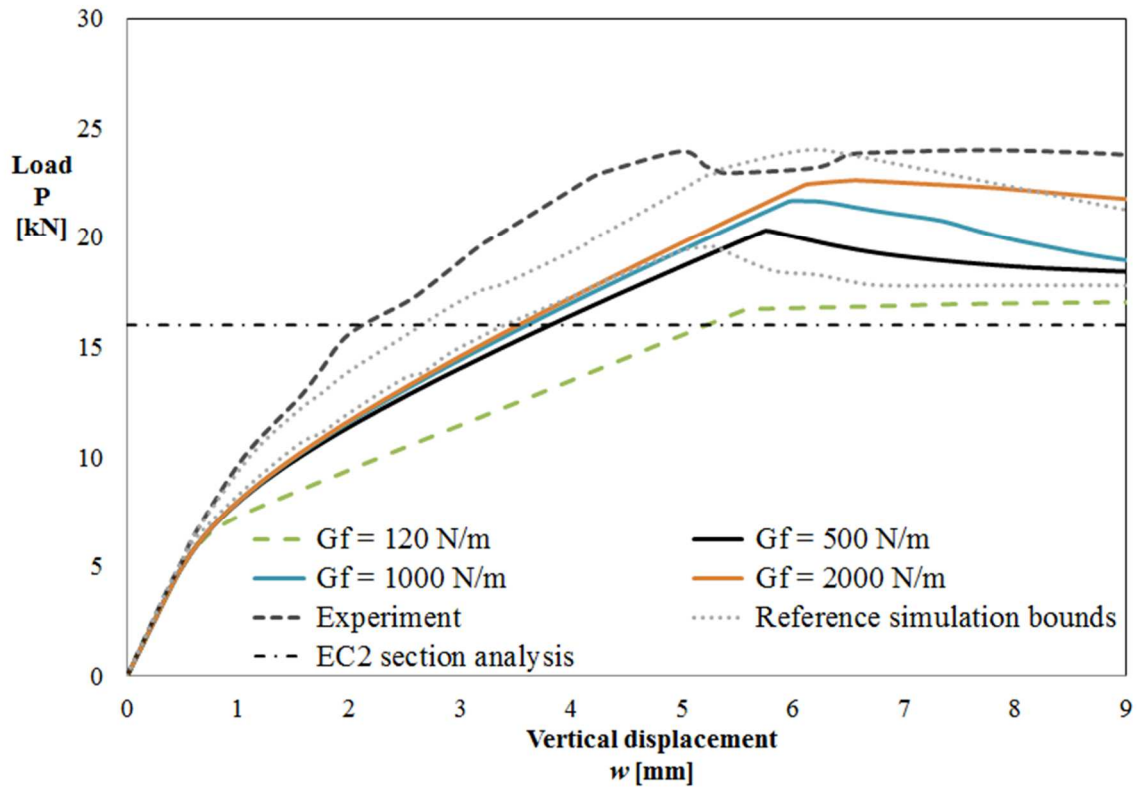


Figure 5.43: Parametric study of Beam 1 with fracture energy as free parameter

Perfect bond is assumed in the current analysis, and it remains unclear how significant its influence is on the outcome. Originally, Rots (1988) states that perfect bond gives rise to diffusion of damage/cracking and that in such situation, where full localisation of primary cracks is hindered, fracture energy is enhanced as compared to plain concrete under fully localised failure. This reasoning, however, is considered to apply to higher reinforcement ratios than  $\rho_s$  of Beam 1, in particular more distributed reinforcement arrangements. On the other hand, and shown in Huber (2006), accounting for progressively weaker bond between concrete and steel only makes the response less stiff in the aforementioned range where dowel effect has been reported as relevant, further achieving a lower peak load.

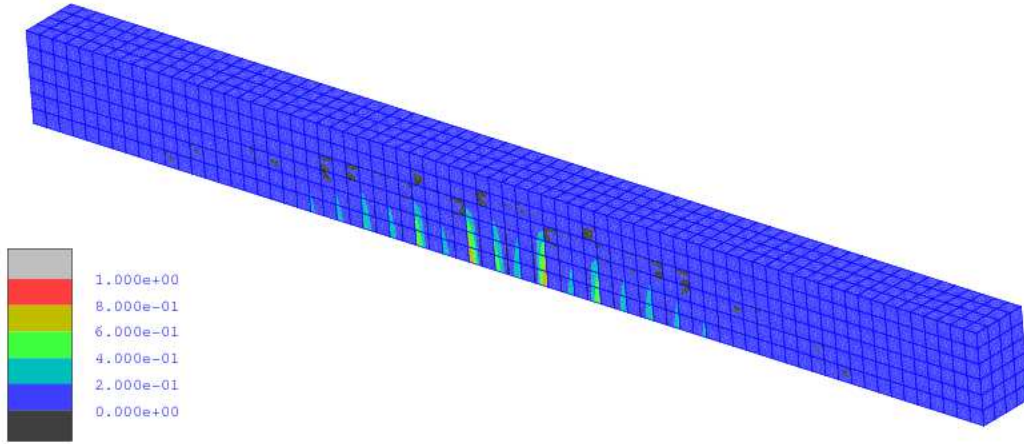


Figure 5.44: Distribution of damage variable  $\omega$  at peak load (displacement  $w = 5.8$  mm)

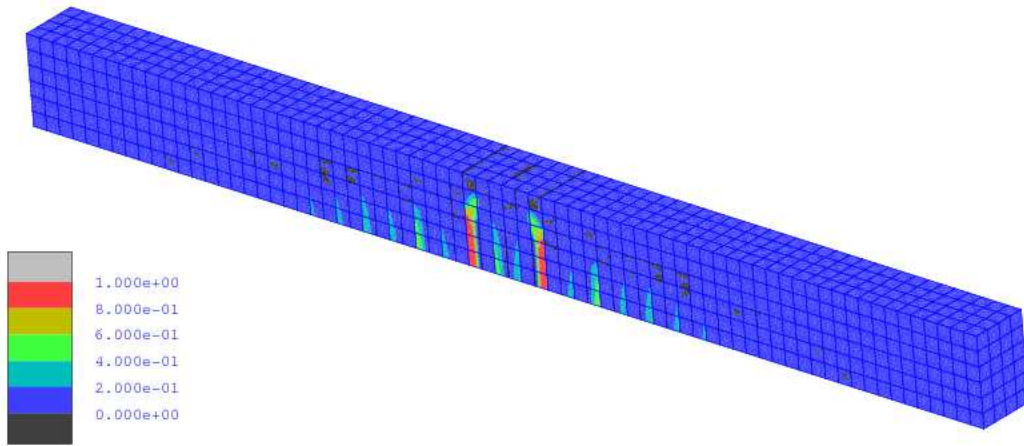


Figure 5.45: Distribution of damage variable  $\omega$  near collapse (displacement  $w = 9.8$  mm)

Figures 5.44 and 5.45 show the scalar damage distribution of Beam 1 at peak load and near collapse. In line with Schütt (2005), the evolution of the damage bands is that of flexural failure, although the mesh induced directional bias encountered in previous examples could be preventing or delaying to some extent the curving of the flexural crack tips.

Additionally, and similar to the PCT-3D test on plain concrete of Section 5.4, Beam 1 is modelled resorting to hierarchic partitioned modelling, dividing the mesh into 3 partitions of similar node ratio. Execution is completed with an approximate reduction of computing time of 40% as compared with the monolithic model, which corroborates the benefits associated to this method in terms of performance.

Lastly, Beam 1 is also analysed with the anisotropic damage model. Figure 5.46 shows the response curve in terms of load vs. displacement resulting from such analysis. Although there are no appreciable differences up to peak load, the softening branch is initially more pronouncedly steep than with isotropic damage. This is related to the fact that the damage models link the equivalent strain to different variables via the damage loading functions. As elaborated in Chapter 3, the isotropic damage model links it to the internal strain-like variable directly entering the scalar damage exponential function, whereas the anisotropic model links it to the trace of the damage tensor. This in turn leads to an incremental relation between scalar damage and equivalent strain, and between the damage tensor and the actual strain tensor, for the isotropic and anisotropic damage model, respectively. The more ‘volumetric’ is the strain state leading to damage, the smaller would the differences be between the isotropic and the anisotropic response. Consequently, it is expected that for greater displacement values  $w$ , the softening curves in Figure 5.46 will tend to coincide.

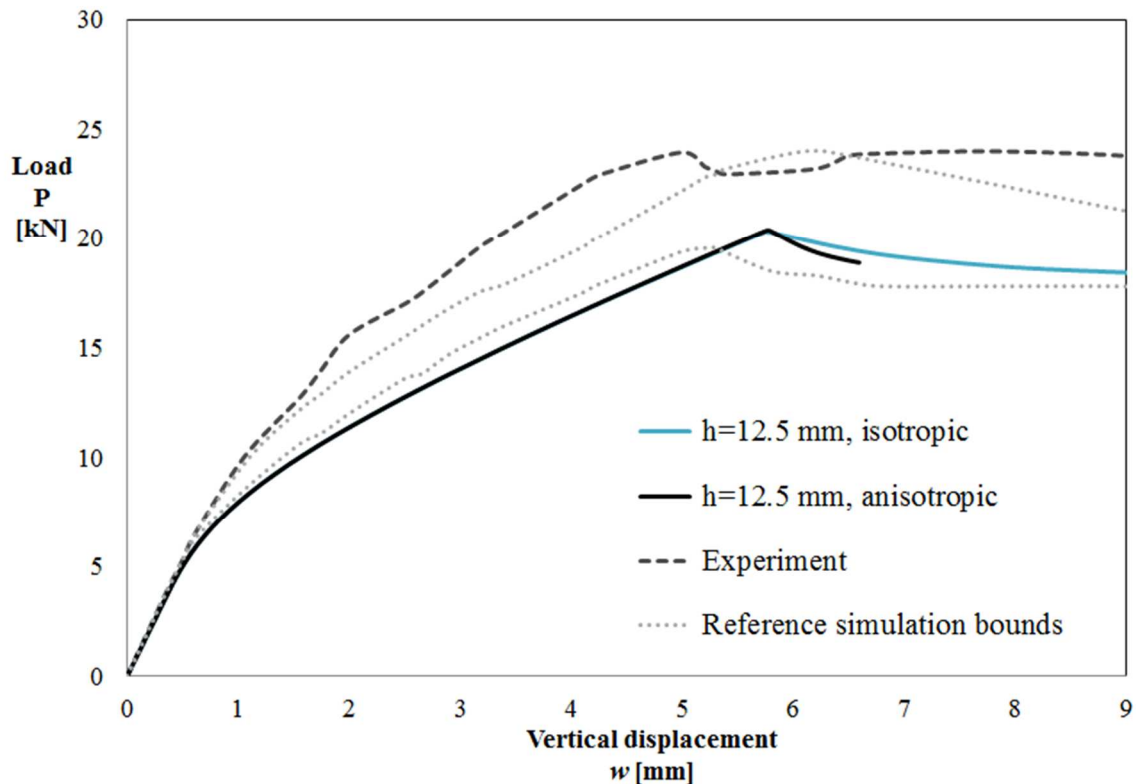


Figure 5.46: Response curve for Beam 1 under isotropic and anisotropic damage

With regard to Beam 2, Figure 5.47 shows its response curve under the same analysis strategy as Beam 1, along with the test curve and the scatter of numerical responses from Suanno (1995), Schütt (2005) and Menrath (1999). As with Beam 1, there is an accentuated

difference between the stiffness measured during testing and its predicted values, which would further reinforce the validity of a greater dowel effect influence for a greater reinforcement ratio.

It is reported in Karihaloo (1992) that failure in this beam abruptly ensued the forming and opening of a diagonal shear crack that initially connected with a debonding crack along one of the bars, further evolving towards the loading plate. This premature bond failure facilitating the shear crack explains the almost immediate drop of the test curve after peak, and possibly entails a shift in the failure mode that would have developed under better bond conditions. Since perfect bond is assumed in all simulations, this scenario cannot be captured, but it is noteworthy that, contrary to Beam 1, in this case the scatter of all numerical responses is of lesser magnitude, with all models predicting fairly homogeneously the peak load and post-peak response.

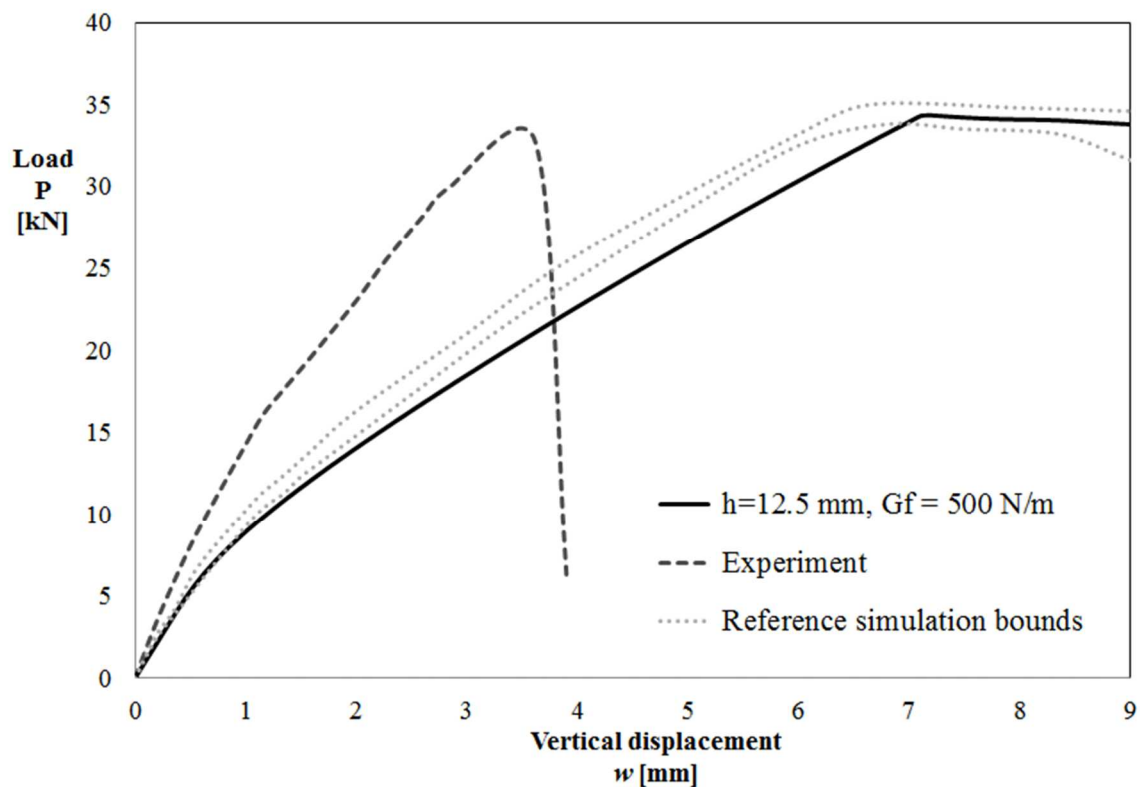


Figure 5.47: Response curve for beam 2, along with the experimental results and the scatter of numerical results by Suanno (1995), Schütt (2005) and Menrath (1999)

Assessing Beam 2 under the Eurocode 2 (2004) guidelines regarding moment-curvature provides an estimate of displacement at peak load reasonably in line with the simulations

(approximately 7 mm). Also, Schütt (2005) refers to Tikhomirov and Stein (1999), where meso-scale analysis tracked a response up to peak load at an approximate displacement value of  $w = 5.8\text{mm}$ , further differing from the failure mode observed during testing.

Figure 5.48 shows the distribution of the scalar damage variable at peak load. As with Beam 1, the displayed propagation of damage bands corresponds to a more ductile failure than the one reported. This can be further confirmed when comparing the damage distribution with the observed experimental crack pattern in Figure 5.49. There is a reasonable fit between damage bands and the primary flexural cracks, but the diagonal shear crack leading to collapse and possibly shifting the failure mode is not captured.

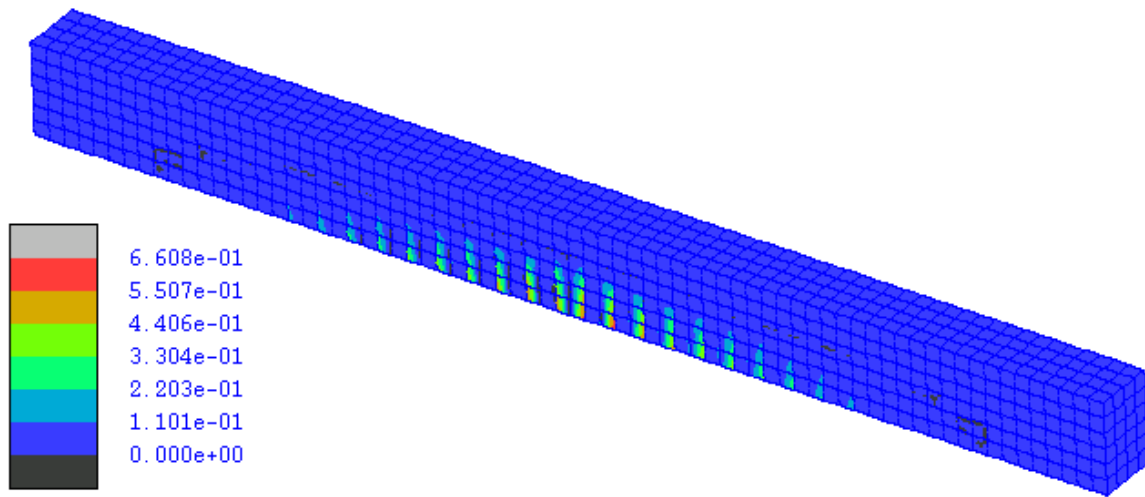


Figure 5.48: Distribution of damage variable  $\omega$  at peak load (displacement  $w = 7.0\text{ mm}$ )

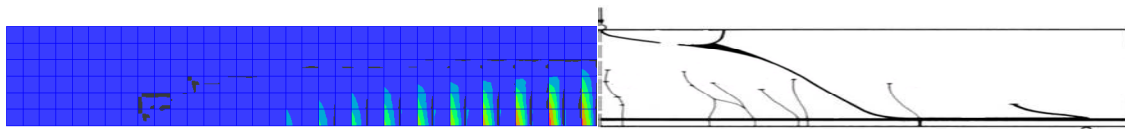


Figure 5.49: Comparison of damage distribution vs. crack pattern (Karihaloo, 1992)

## 5.7 Conclusions

The numerical examples presented and discussed in this chapter cover benchmark tests of different structural behaviour, and prove to constitute a reasonable framework in which to assess the validity of the enhanced concrete material model and the proposed embedded reinforcement approach.

The significant computational convenience of treating the characteristic element size  $h$  as a fixed parameter, as opposed to considering it a local internal variable based on a projection method as described in Chapter 3, is confirmed with the notched three-point bending simulation. For more irregular mesh regions prone to contain a damage band, it would be preferable to define a finite set of values for  $h$  and distribute them based on mesh morphology considerations. Although less systematic and sensitive to errors by the analyst, the benefits in performance justify this approach.

Simulations of the torsion beam show that a convenient mesh morphology may alleviate the effects of mesh-induced directional bias. Hence, despite the loss of ellipticity at the global level and the consequent loss of solution uniqueness, it is still possible for the damage band to propagate in the correct direction provided that it pertains to the directions made available by the mesh main orientations. In any case, it is also shown that even biased solutions dissipate approximately the same amount of energy.

Applying localisation analysis to the CDPM, as per the corresponding elaborations in Chapter 3, does not contribute noticeably to overcome mesh-induced directional bias if the appropriate damage propagation direction is not facilitated by the mesh orientation. Furthermore, the need for tracking the potential singularity of the localisation tensor for each sample point severely hinders performance.

The extension of the CDPM to anisotropic damage does not noticeably alter the global response in terms of peak load prediction or damage distribution, although a minor increment in dissipated energy is noted for the same mesh type and characteristic element size. This is further investigated in the larger scale case study of Chapter 6.

Resorting to hierarchical partition modelling, particularly under dynamic analysis of the PCT-3D specimen, is shown to improve performance, allowing for a significantly larger output for the same computing time as a *monolithic* model. This confirms the capabilities of this numerical technique, which is corroborated by the unnotched three-point bending reinforced concrete test simulation. Shifting from static to dynamic analysis, however, does not entail benefits regarding the mesh-induced directional bias.

The uniaxial compression test simulations for a cube and a cylinder corroborate the capability of the model to reflect damage propagation arising under compressive states. In these circumstances, however, particularly if damage tends to be diffuse, the choice of a fixed parameter representing a characteristic element size becomes less intuitive.

The reinforced concrete beam simulations highlight the importance of the fracture energy estimation, particularly for laboratory-size specimens. In its current form, the model seems to display a strong sensitivity to the presence of reinforcement bars with perfect bond, with a tendency to necessitate greater values of fracture energy than code estimations to dissipate energy correctly. This feature can be associated to the transition from localised to diffuse damage, a trend reinforced by the perfect bond assumption, but is not entirely consistent here. Further insight into this sensitivity is given by the case studies of Chapter 6.

# CHAPTER 6

## Major case studies

### 6.1 Introduction

The material model for concrete and reinforcing steel, as implemented in the nonlinear Finite Element program ADAPTIC (Izzuddin, 1991), is tested in Chapter 5 in the framework of benchmark simulations for validation purposes. Following the disquisitions and conclusions presented there, the current chapter aims at testing the validated model by means of case studies of considerably larger scale, outside the usual scope of design codes. As elaborated in subsequent sections, the increase in domain dimensions has relevant consequences in the simulation outcome, which pose numerical challenges not encountered in previous chapters.

As with the benchmark simulations of Chapter 5, all elements forming the 3D mesh are of quadratic order with full Gauss integration by default. A fixed characteristic length parameter  $h$  is adopted throughout, and no additional localisation analysis module is used. Both static and dynamic analyses are resorted to, with isotropic and anisotropic damage, and their results are discussed separately hereafter.

## 6.2 Case 1

### 6.2.1 Geometric description and test setup

The first case study is based on the prediction contest organized by the University of Toronto (Collins *et al.*, 2015) to assess the current ability of engineering practice and academia to estimate the shear resistance of structural members of very significant thickness. To this end, a 250 mm wide strip representative of a 4 m deep simply supported slab was cast and tested under an eccentric point load, as schematically shown in Figure 6.1, and served as benchmark against which to compare the predictions. The span length between supports is 19 m, divided by the applied load in two unequal spans of 7 m and 12 m, to the west and east side of the load, respectively. The west span contains shear reinforcement as per the minimum provisions of ACI 318 (1995), resulting in 5 headed studs of 300 mm<sup>2</sup> cross sectional area, whereas the longer east span contains no shear reinforcement. Longitudinal reinforcement comprises a single top layer of 3 20M bars (corresponding to a diameter of 19.5 mm) and a triple bottom layer of 9 30M bars (corresponding to a diameter of 29.9 mm). Further details regarding the specimen geometry, support conditions, test setup and loading and measuring procedures can be found in Collins *et al.* (2015).

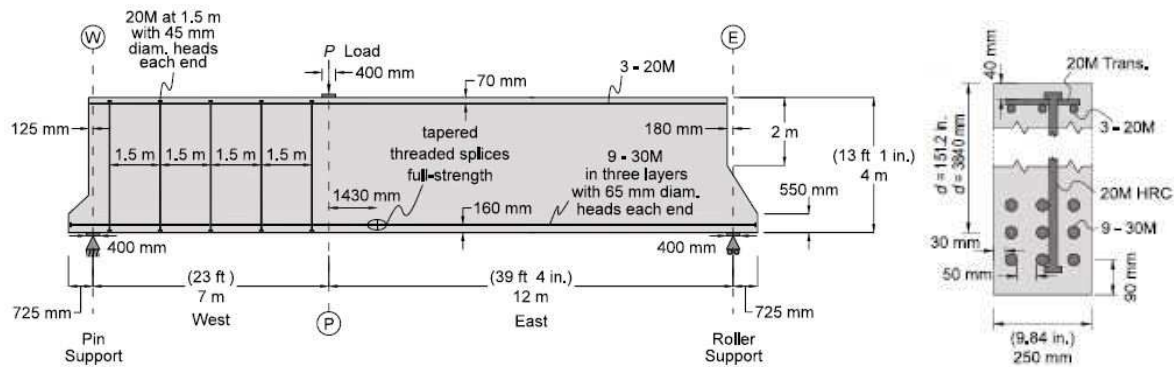


Figure 6.1: Geometry and experimental setup of the very thick slab strip (Collins *et al.*, 2015)

### 6.2.2 Mesh definition and parameters

Only the uniaxial compressive strength (40 MPa) and the maximum aggregate size (14 mm) are provided in the original report, along with the yield stress values of reinforcement (573 MPa for 30M bars and 522 MPa for 20 M bars). Hence, CEB-FIP Model Code (1990) is used to estimate the remainder of necessary material parameters for concrete, whilst for reinforcing steel usual values from the technical literature are adopted, leading to the following set of parameters:

$$\text{concrete} \begin{cases} E = 34100 \text{ MPa} \\ \nu = 0.2 \\ f_c = 40.0 \text{ MPa} \\ f_t = 3.0 \text{ MPa} \\ G_f = 78 \text{ J/m}^2 \end{cases} \quad \text{steel} \begin{cases} E_s = 200000 \text{ MPa} \\ H = 1510 \text{ MPa} \end{cases}$$

The initial mesh considered for analysis comprises 4028 20-noded hexahedrons and 20 additional 15-noded pentahedrons (wedges), to accommodate the protrusions at both ends of the slab strip. 22 straight macro-segments account for as many bars, representing the longitudinal and transverse reinforcement. Both element sets are depicted in Figure 6.2. Given the mesh overall regularity, it is decided to take the characteristic element size as  $h = 140 \text{ mm}$ . To reflect the inclusion of external steel frames providing out-of-plane stability in the real test, the lines marked in black in Figure 6.2 are restrained in that direction.

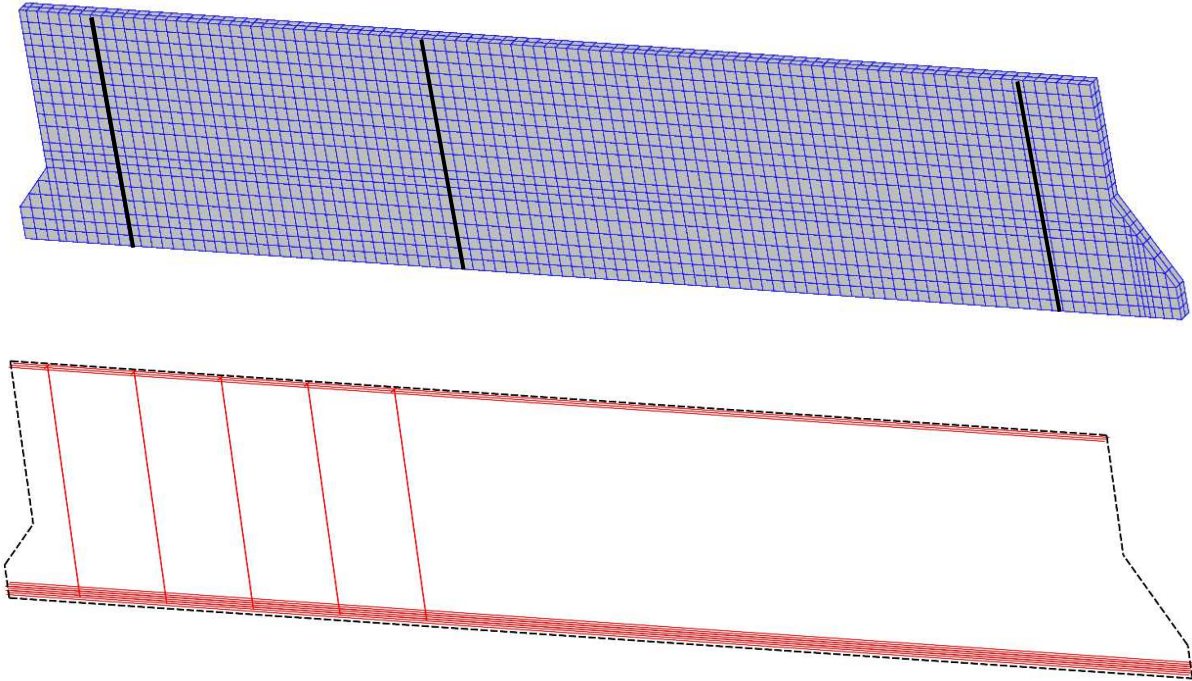


Figure 6.2: Structured mesh adopted for analysis (top) Concrete mesh  
(bottom) Reinforcement macro-segments

Originally, the scope of the contest included not only the prediction of the peak load, associated vertical displacement and crack pattern at failure of the east span (as shown in Figure 6.3 from the test measurements) but also their equivalents upon repairing of the east span via external post-tensioned threadbars and further loading until failure of the west span.

The current simulation, however, concerns only the first stage and hence only failure of the east span is considered.

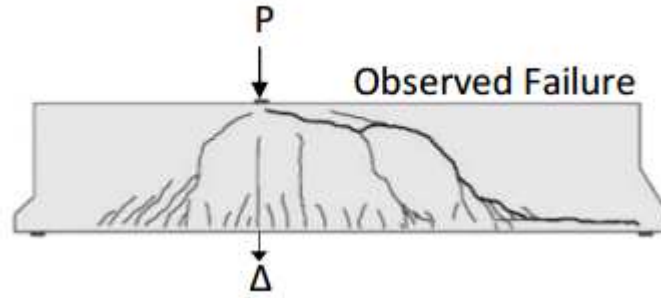


Figure 6.3: Crack pattern at failure of the east span (Collins *et al.*, 2015)

### 6.2.3 Static analysis

Following application of a distributed element load to represent the significant effect of self-weight, a uniformly distributed load across the area of the loading plate is translated into nodal forces for an initial load control stage. Subsequently, and given the great contrast between the expected localisation process zone and the overall dimensions of the specimen, it is decided to discard an arc-length strategy in favour of a series of indirect displacement control stages, following relative displacements of relevant nodes across the expected damage bands, similar to crack mouth opening displacements (CMOD) in fracture processes. As an auxiliary measure, some analyses are carried out with an overlain level of elements, of the same type and order as the original mesh and associated to a linear elastic material model with parameters:

$$\text{concrete} \begin{cases} E_2 = 0.01 \text{ MPa or } E_3 = 0.0001 \text{ MPa} \\ \nu_2 = 0.2 \end{cases}$$

whereby  $E_2$  and  $E_3$  are used with static and dynamic analysis, respectively. This set of parameters is aimed at allowing for a residual element stiffness upon extensive damage evolution, as for the isotropic damage model all stiffness components decrease proportionally to  $(1-\omega)$ . For scalar damage values close to unity this may lead to the bottom layers (Figure 6.2) losing integrity, artificially reflecting a failure mode closer to splitting along the bottom reinforcement layer.

### 6.2.3.1 Isotropic damage

Figure 6.4 shows the response curve in terms of load  $P$  vs. displacement  $\Delta$  resulting from static analysis and isotropic damage, alongside the winner prediction of the contest, reported by Červenka *et al.* (2016). Aside from an overestimation of the elastic modulus, convergence difficulties do not allow the iterative procedure to advance until the reaching of peak load, and along the tracked solution path snap-backs must be overcome, coinciding with primary crack formation. This can be corroborated when observing the scalar damage distribution corresponding to the last converged output in Figure 6.5, where 2 major damage bands develop.

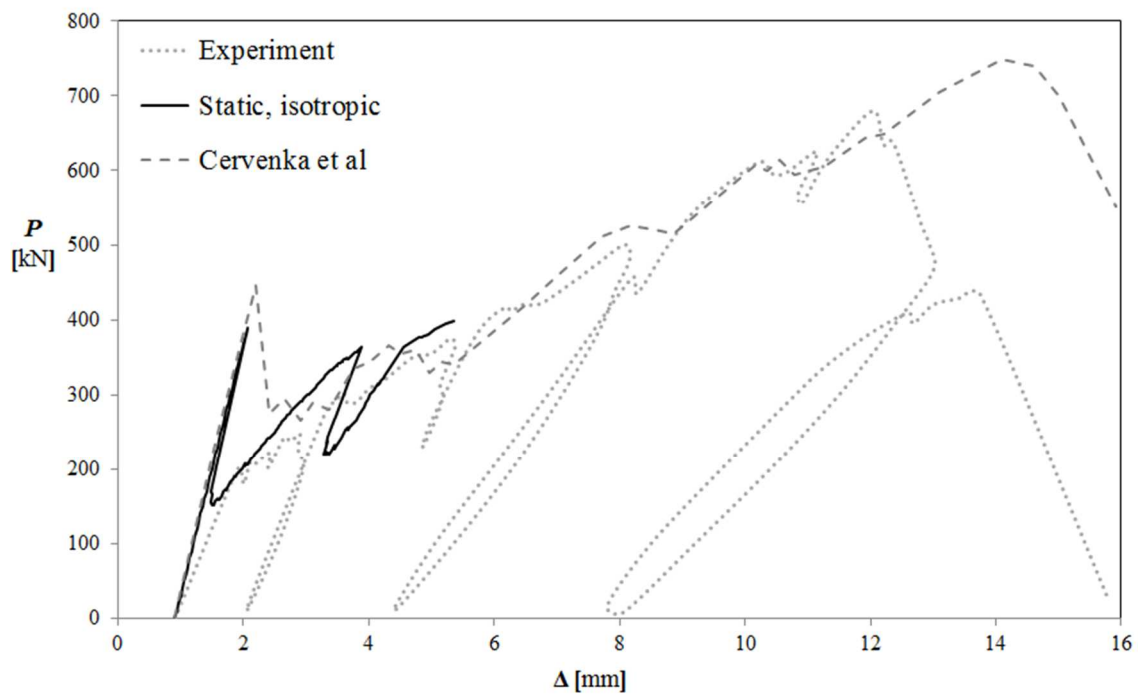


Figure 6.4: Response curve of the slab strip under static analysis with isotropic damage

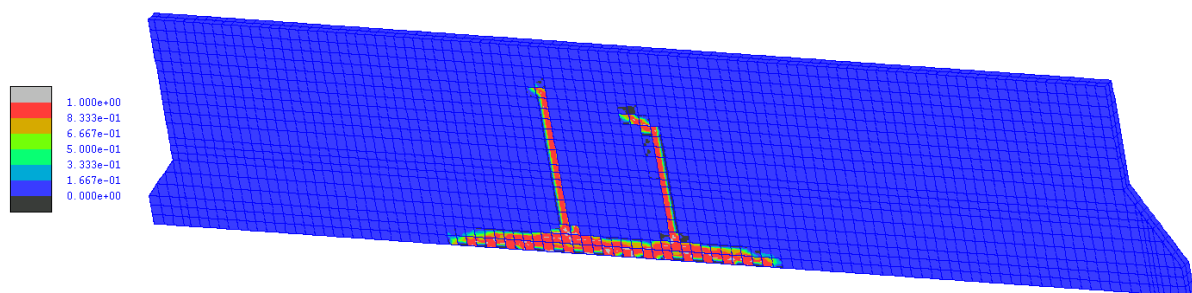


Figure 6.5: Scalar damage  $\omega$  distribution under static analysis ( $\Delta \approx 5.4$  mm)

Although the experimental curve in Figure 6.4 represents an average trend, where oscillations have been smoothened out, the pronounced drop upon onset of cracking was not observed in the test. Whilst it is possible that restrained shrinkage reduced the cracking load in the test, as is generically suggested in Pryl and Červenka (2016), it is unlikely that a reinforcement ratio  $\rho = 0.75\%$  would attain a reducing effect of 50%. Illustratively, a conservative application of Eurocode 2 (2004) provisions for total shrinkage strains at 28 days on the adopted set of material parameters leads to a value below 140 microstrains. For a tensile strut, this can be shown to reduce the cracking load by less than 10% (Bischoff, 2001). Hence, this option is not pursued further. It was initially believed that the fracture energy could be underestimated and hence be giving rise to the initial abrupt snap-back. To investigate this, a parametric study was carried out, letting parameter  $G_f$  vary as  $\{2G_f^0, 5G_f^0, 10G_f^0\}$ , with  $G_f^0$  being the original estimation of fracture energy based on CEB-FIP Model Code (1990). The resulting response load vs. displacement curves are shown in Figure 6.6.

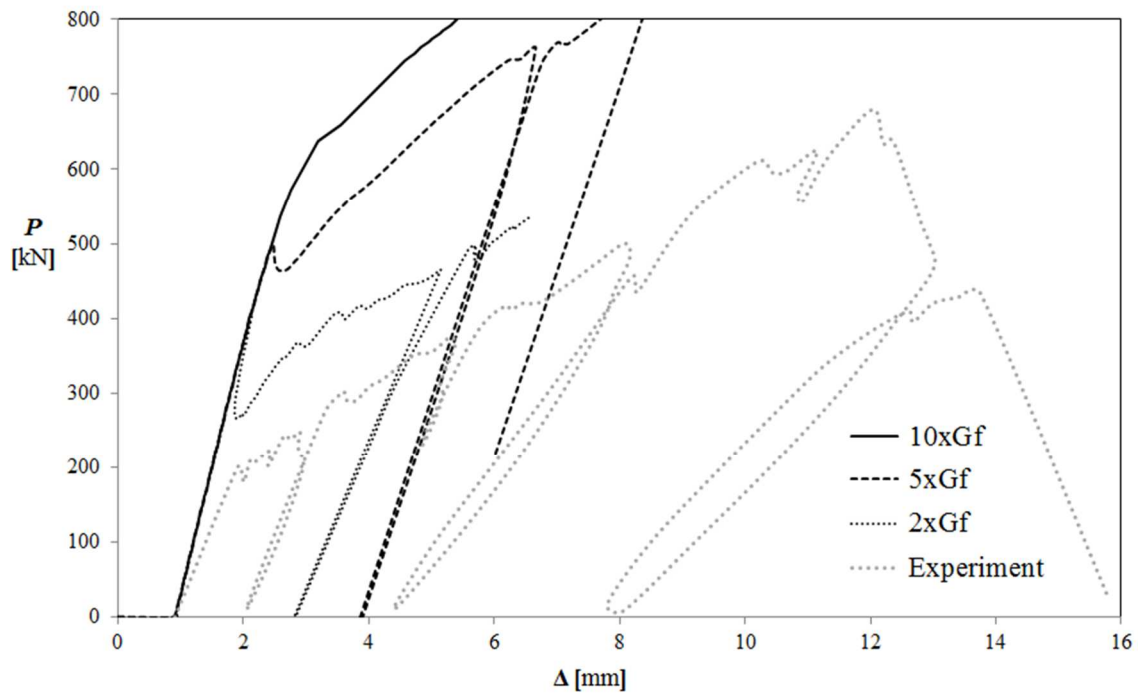


Figure 6.6: Response curves of the parametric study on  $G_f$

It is noteworthy that for greater fracture energy values, which not only accentuate the plastic flow but also delay damage evolution, there is a progressive reduction in the initial drop, evolving from a snap-back to a regular smooth transition between the initial elastic branch

and the pre-peak cracked/damaged branch. Moreover, Figure 6.6 indicates that  $G_f^0$  is indeed an adequate estimate of the fracture energy. The crack patterns (or scalar damage distributions) associated to  $\{2G_f^0, 5G_f^0, 10G_f^0\}$ , shown in Figure 6.7, are also of interest. As discussed in Chapter 3, the non-associativity of the concrete plastic flow entails that onset of damage and localisation may precede each other indistinctly, depending on the case.

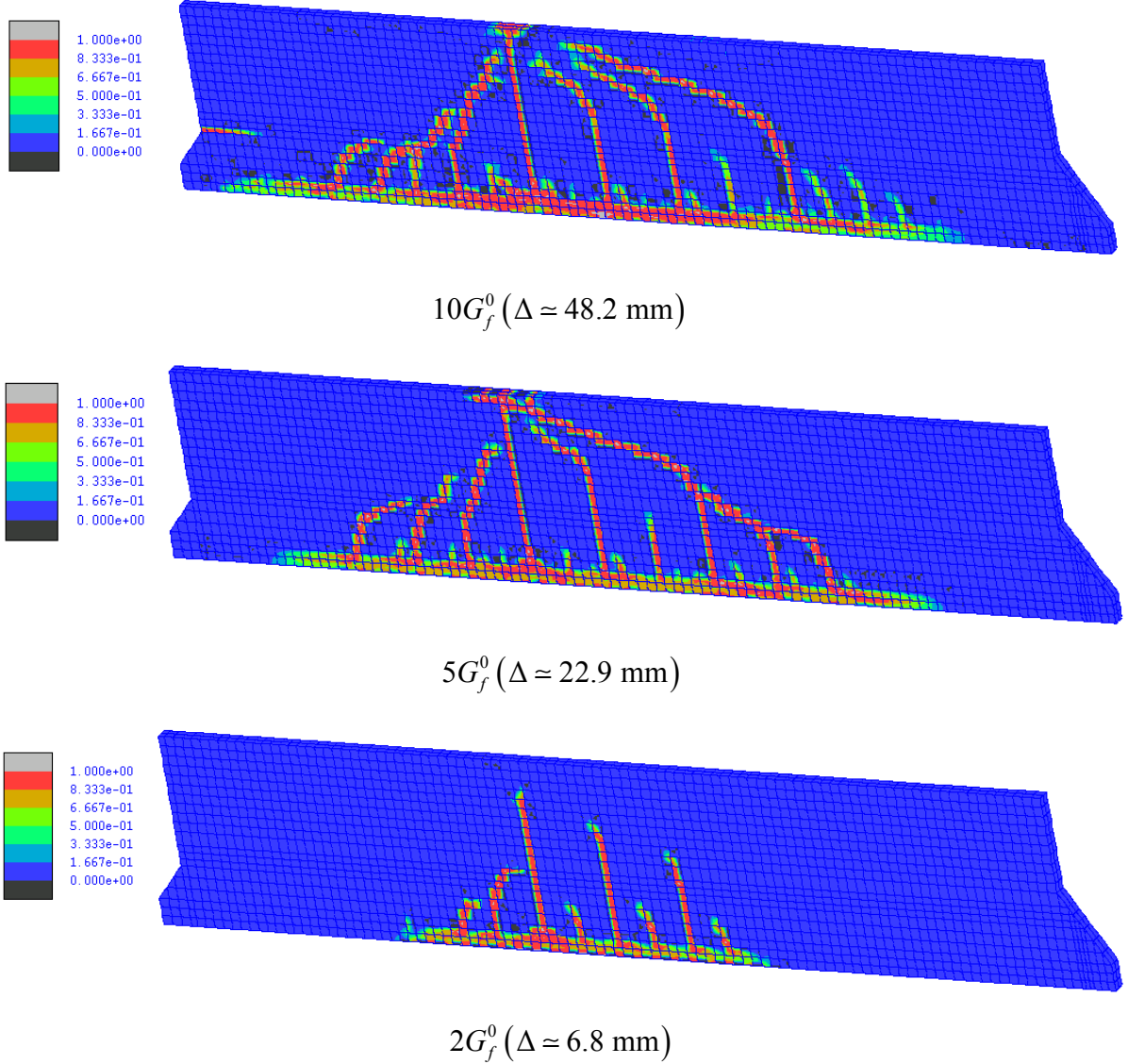


Figure 6.7: Scalar damage  $\omega$  distribution for different values of  $G_f$

Illustratively for  $\{G_f^0, 10G_f^0\}$ , Figure 6.8 shows that onset of localisation succeeds onset of damage, the latter being unaffected by the increase of fracture energy. It is thus the onset of localisation that gets delayed alongside the evolution of damage. As can be seen for  $10G_f^0$  in

Figure 6.7, this facilitates the development of damage bands for greater displacement values that are in good agreement with the observed crack pattern, depicted in Figure 6.9.

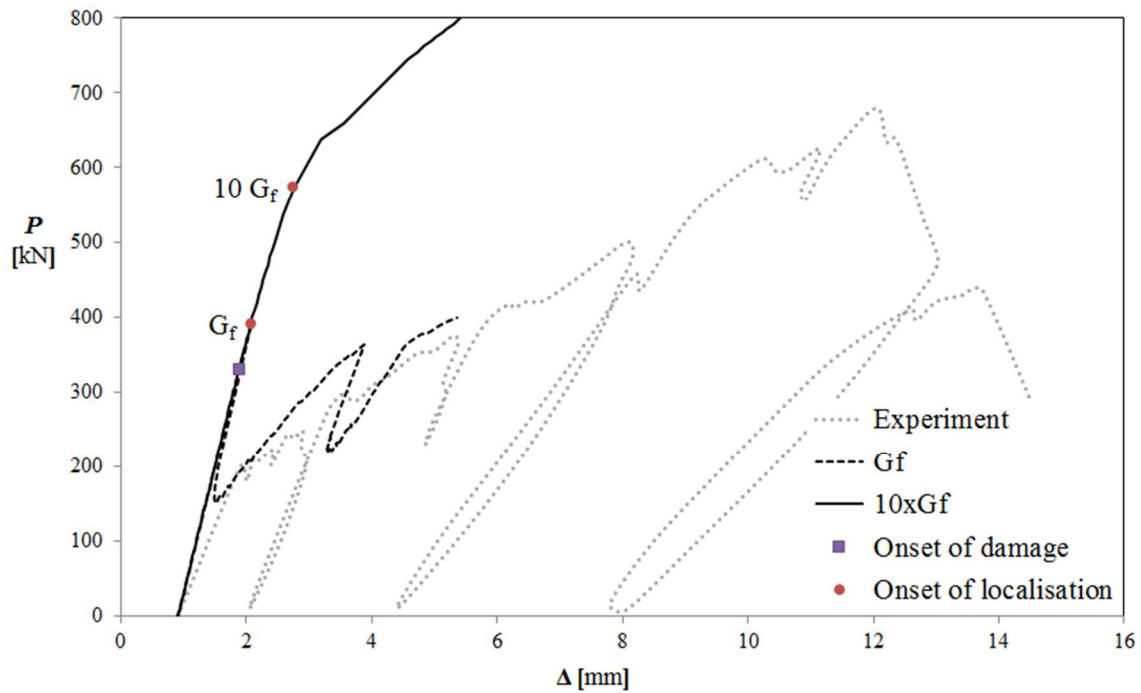


Figure 6.8: Response curves marking onset of damage and first primary crack

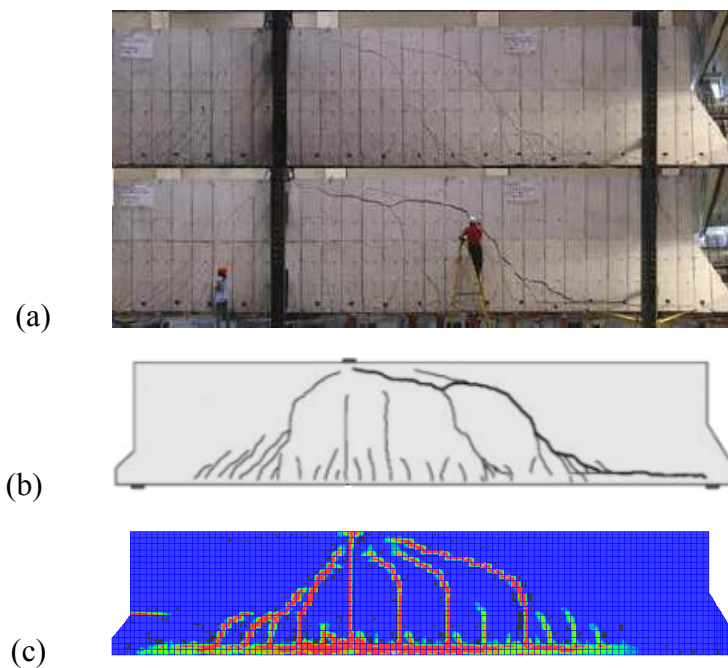


Figure 6.9: (a) Test crack pattern at failure load  $P = 685$  kN (top) and at post-peak  $P = 433$  kN (bottom) (b) Schematic observed crack pattern at post-peak (Collins *et al.*, 2015) (c) Damage distribution at post-peak for  $G_f = 10G_f^0$

Despite the loss of ellipticity in the global boundary value problem, the displayed pattern does not suffer from a strong mesh-induced directional bias, which suggests that this effect, once triggered alongside localisation, does evolve in a quantifiable manner and may be delayed despite the great plastic deformations. Figure 6.10 further corroborates the correspondence between the observed failure mode and the one reproduced by  $G_f = 10G_f^0$ , displaying the distribution of the longitudinal nominal stress in concrete at peak and post-peak load levels. The strut developed in the east span (Figure 6.10 bottom) approximates well the observed diagonal crack connecting the loading plate with the debonding crack towards the east support.

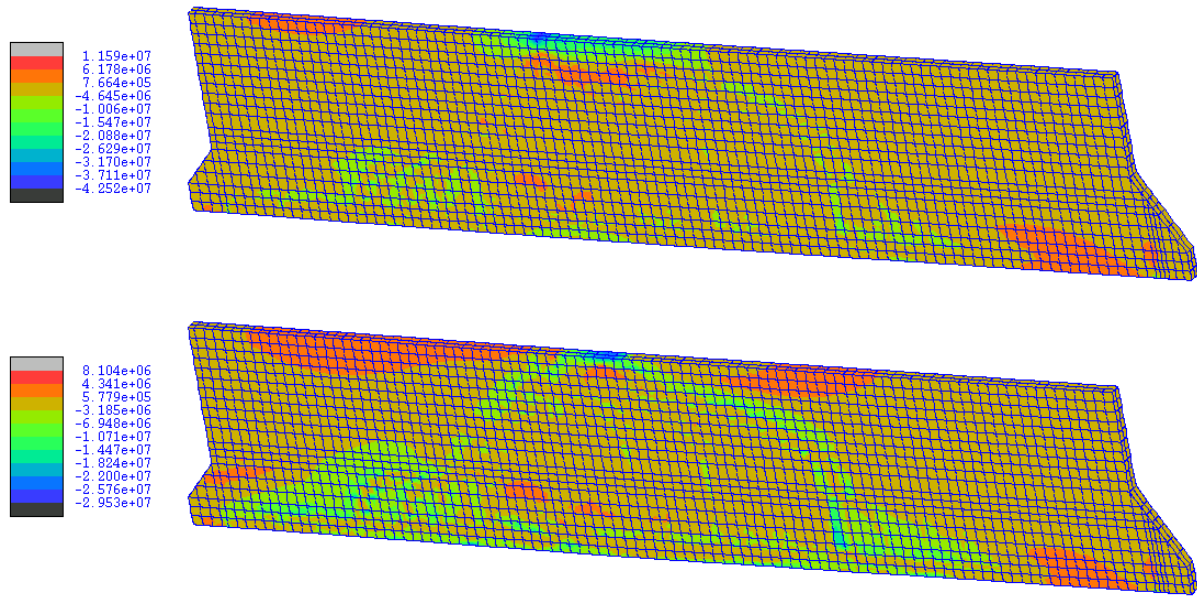
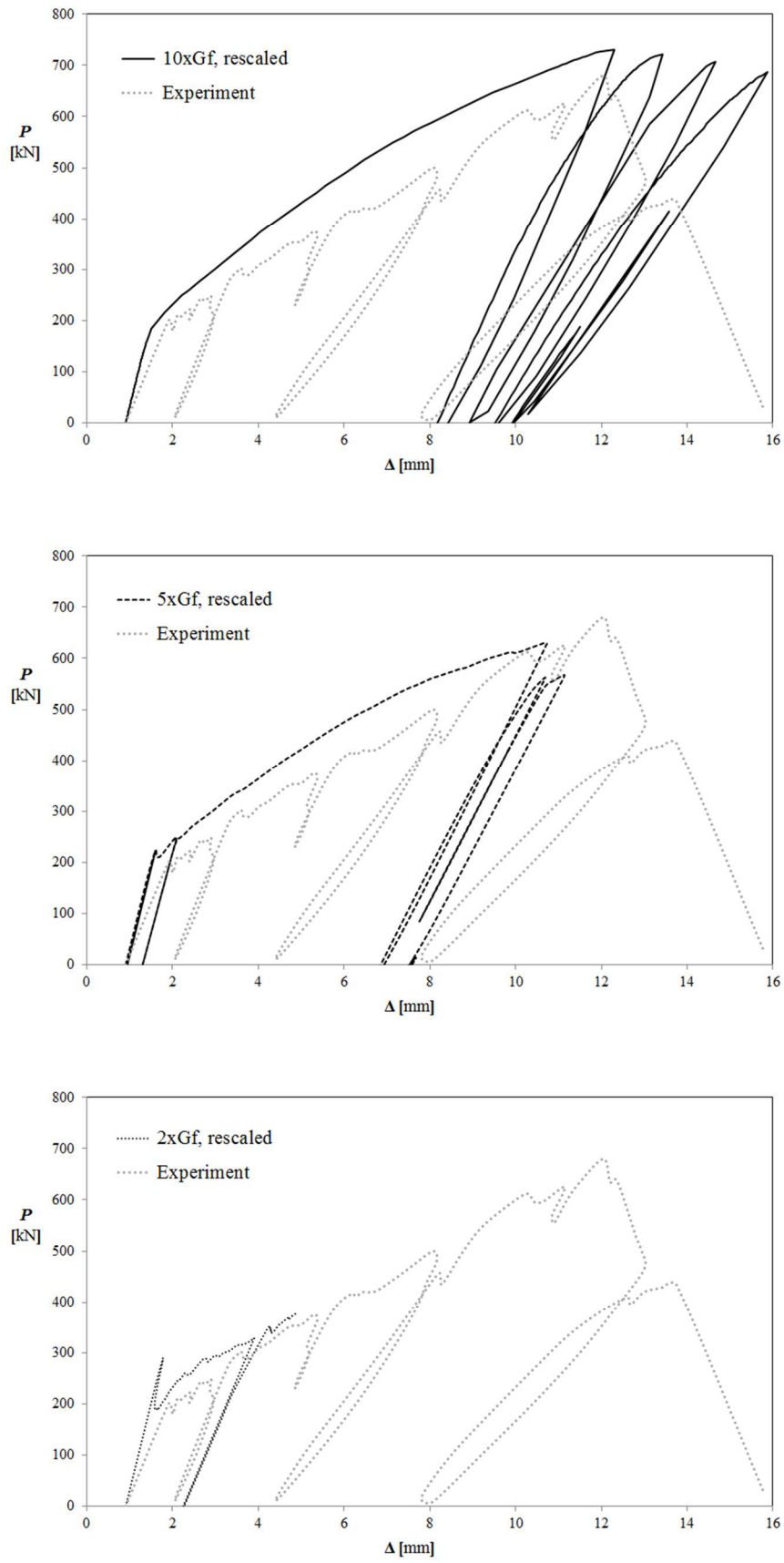


Figure 6.10: Distribution of  $\sigma_x$  for  $G_f = 10G_f^0$  and (top)  $\Delta \approx 36.8$  mm  
(bottom)  $\Delta \approx 48.2$  mm

Interestingly, an indirect approximate way of assessing the consistency of the response curves resulting from  $\{2G_f^0, 5G_f^0, 10G_f^0\}$  is by applying a rescaling factor of  $\{1/\sqrt{2}, 1/\sqrt{5}, 1/\sqrt{10}\}$  to both load  $P$  and displacement  $\Delta$ , so that the work performed during the loading process is reduced in roughly the same proportion as the fracture energy is augmented. This is vaguely based on the rescaling applied to the tensile strength when the characteristic length  $h$  surpasses the threshold  $h_{cr}$  defined in Chapter 3, following Bažant (1986). Upon rescaling, the response curves depicted in Figure 6.11 are obtained.

Figure 6.11: Rescaled response curves for  $\{2G_f^0, 5G_f^0, 10G_f^0\}$

Although they cannot be used themselves directly to obtain a value of peak load and associated displacement, they constitute additional indicators that the amount of dissipated energy arising from the assumed value for  $G_f^0$  is reasonable. Once corroborated that the fracture energy as estimated from CEB-FIP Model Code (1990) is not in itself the reason for the sudden initial drop in the response curve, attention is focused on the assumed material homogeneity. As reported in Červenka *et al.* (2016), maintaining constant values for the fracture related parameters (tensile strength  $f_t$  and fracture energy  $G_f$ ) across a specimen of such great dimensions is unrealistic and makes the model unable to reflect properly the onset of localisation. It is argued by these authors that, whilst in reality it is more likely that scattered imperfections in early micro-cracking coalesce progressively, a homogeneous field of material properties gives rise to a sudden macro-crack, leading to an unstable response. In order to investigate if the current model accommodates this effect, the 2 aforementioned parameters  $(f_t, G_f)$  are transformed into random variables, with their initial estimations as mean values and following a normal distribution with a coefficient of variation 0.2. Contrary to Červenka *et al.* (2016), no correlation lengths are defined, which is physically less intuitive. The reason is twofold: the current investigation is not a proper probabilistic study *per se*, as the required number of analyses to constitute a reliable sample should be greater, and assuming no correlation maximises the scatter, hence effectively representing an upper bound. With such considerations, Figure 6.12 shows a sample of response curves under different  $(f_t, G_f)$  spatial distributions.

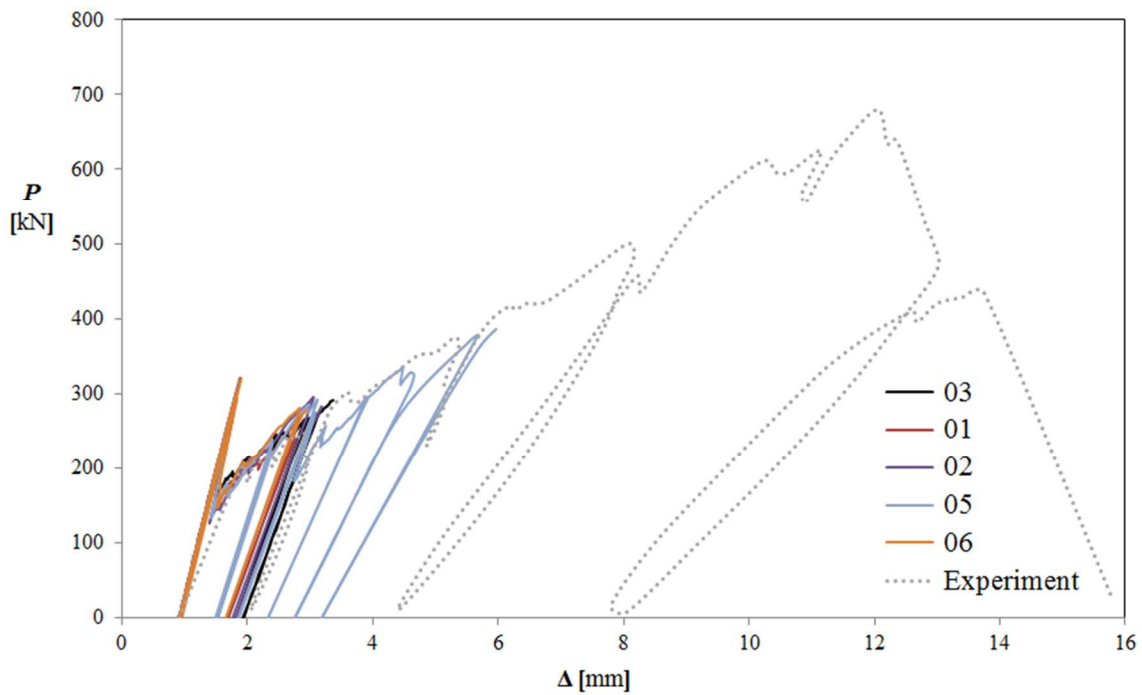


Figure 6.12: Response curves under different spatial random distributions

Although the various responses are tracked insufficiently, as the sequential indirect displacement control stages cannot enable analysis to reach the peak load, all cases accommodate the initial stages of macro-cracking. The sudden initial drop is indeed sensitive to the scatter in  $(f_t, G_f)$ , since depending on the random distribution it may decrease significantly, as illustratively shown in Figure 6.13 for the case with the least abrupt transition.

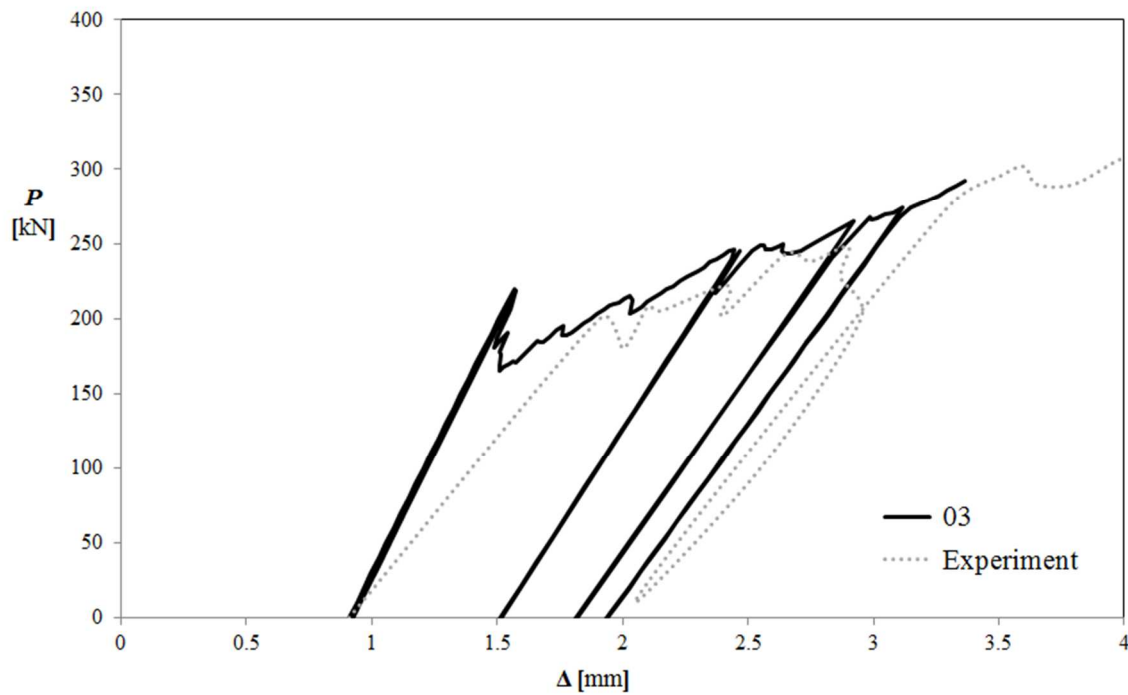


Figure 6.13: Response curve of random distribution with alleviated initial drop

The damage pattern of random spatial distributions 03 (smallest initial drop) and 05 (longest response tracking) is shown in Figure 6.14. When comparing against the pattern of Figure 6.5, stemming from a homogeneous material distribution, it is noteworthy that the order of macro-crack formation displays sensitivity to the spatial distribution of material properties. In both distributions of Figure 6.14, onset of macro-cracking in the west span precedes the formation of the second vertical crack in the east span, which suggests, particularly with distribution 03 in mind, that a similar sequence might have taken place in the real test. Even for the damage pattern of Figure 6.5, however, the amount of dissipated energy is reasonable. Hence, as long as the crack pattern at failure and the dissipated energy are predicted reasonably without changing the failure mode, it is considered that a full probabilistic analysis is not required here and material homogeneity can be maintained.

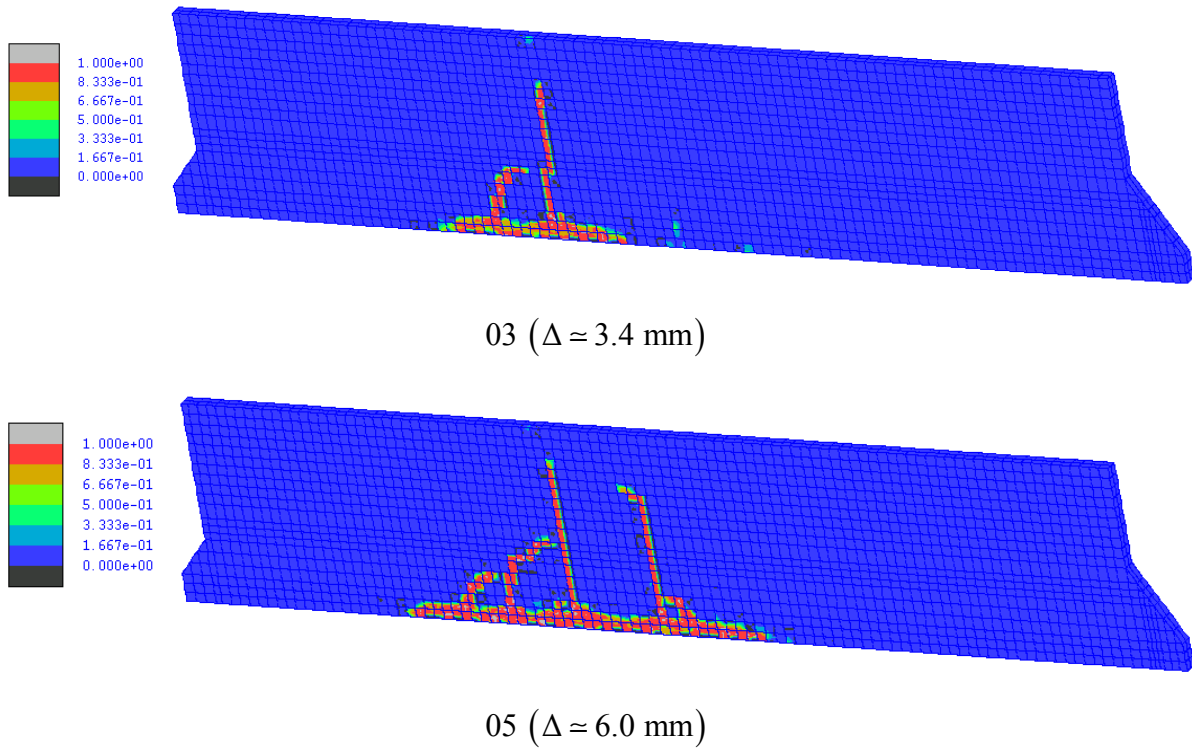


Figure 6.14: Scalar damage distribution  $\omega$  for random distributions 03 and 05

### 6.2.3.2 Anisotropic damage

Resorting to anisotropic damage under the same set of material parameters leads to similar difficulties in the progress of the iterative procedure, the indirect displacement control stages not being enough to reach the peak load (Figure 6.15).

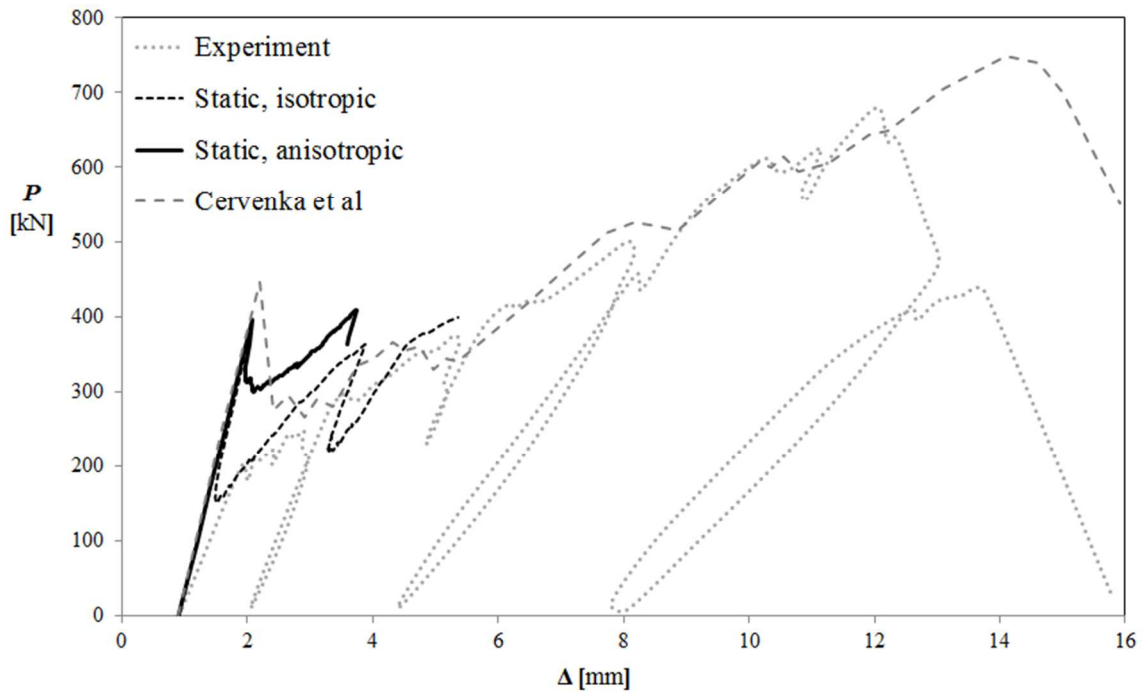


Figure 6.15: Response curve with isotropic and anisotropic damage

As expected, the sudden initial drop is present, following the assumed material homogeneity. The response curve of Figure 6.15 can only advance past the initial snap-back, corresponding to the formation of the first macro-crack in the cross-section of load application, depicted in Figure 6.16.

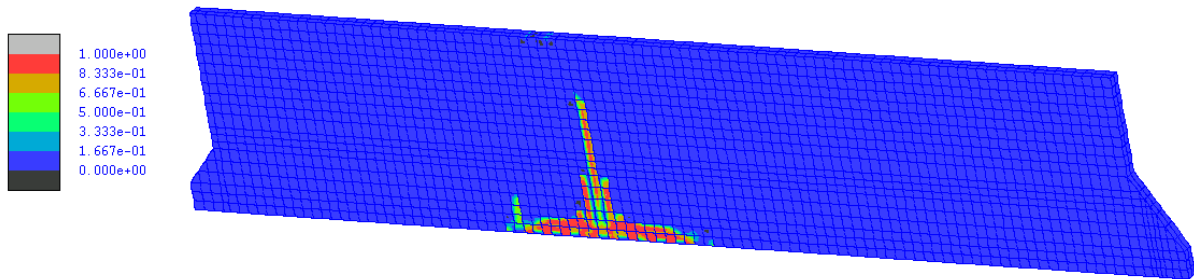


Figure 6.16: Distribution of the first principal value of damage tensor  $\omega$  ( $\Delta \approx 3.7$  mm)

In the stages following onset of macro-cracking, however, Figure 6.15 shows a noticeable increase of stiffness as compared to the isotropic damage response. This increase is also sustained when analysing the random spatial distribution 03 (Figure 6.17), whereby an even more smooth transition from the elastic to the post-cracking branch is achieved.

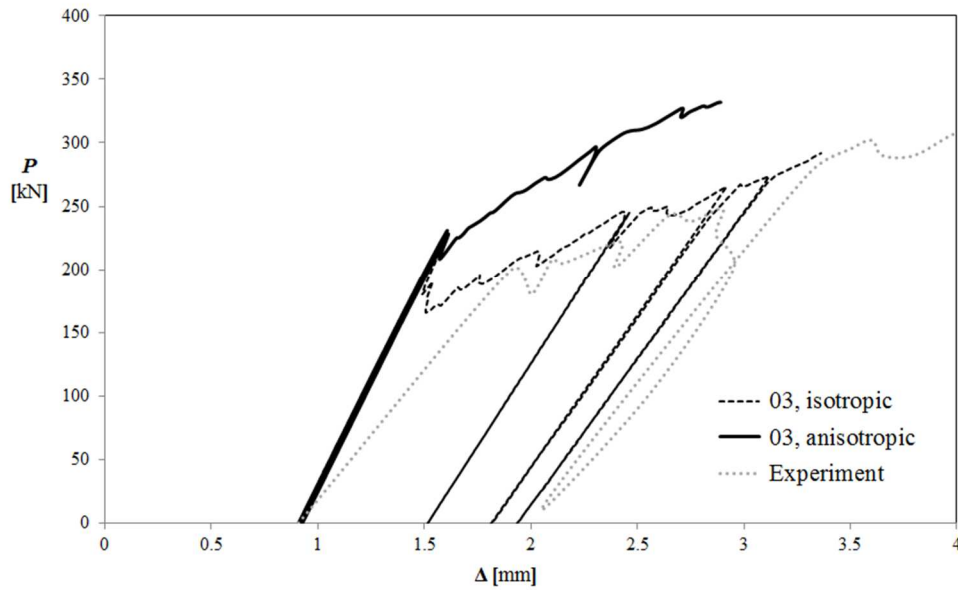


Figure 6.17: Response curve of random distribution with isotropic and anisotropic damage

Such feature, though apparently favourable from the probabilistic perspective of the investigation regarding the initial drop upon cracking, is deemed to emerge from the stress locking phenomenon noted in Chapter 2. This spurious transfer of stresses would explain why the first flexural macro-crack in Figure 6.16 expands to the adjacent vertical layers. As a result, the apparent increase in stiffness must also be considered of spurious nature. To illustrate this, Figure 6.18 shows the evolution of two stress components as evaluated in a sample point of an element embedded in the primary central crack: the longitudinal normal stress and the in-plane shear stress component.

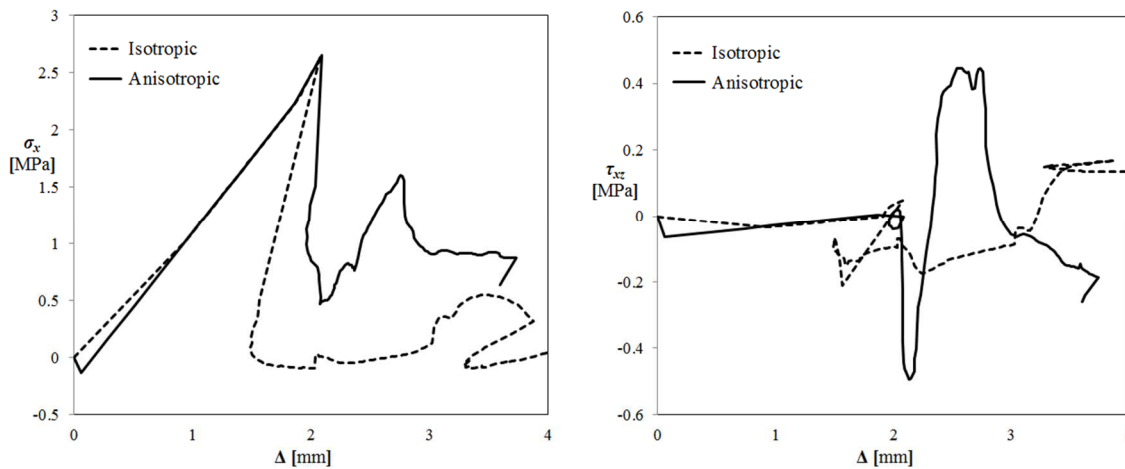


Figure 6.18: (left) Longitudinal stress and (right) In-plane shear stress, at a Gauss point inside the flexural macro-crack

The shear stress inside the damage band is significantly larger in magnitude in the case of anisotropic damage, in turn leading to greater normal stress. Recalling from Chapter 3 that nominal shear stress is obtained by affecting its effective counterpart by different damage components in principal base, it follows that slower damage evolution in different directions leads directly to a greater transfer of spurious stresses. The scalar damage model, whilst still sensitive to these artificially transferred shear stresses in effective stress space, can overcome its effect by applying to all components the same damage parameter.

#### 6.2.4 Dynamic analysis

In order to further assess the response curve and the damage distribution as compared to the experimental measurements, the same mesh and set of material parameters are used with explicit dynamic analysis. As with the notched specimen PCT-3D of Chapter 3, a linear curve is defined in order to induce a displacement under constant velocity ( $v_0 = 1 \text{ cm/s}$ ) in the nodes underneath the loading plate. The integration scheme is of the Hilber-Hughes-Taylor type with parameters:

$$\begin{aligned}\alpha &= -\frac{1}{3} \\ \beta &= \frac{(1-\alpha)^2}{4} \\ \gamma &= \frac{1-2\alpha}{2}\end{aligned}$$

The dynamic response curves and damage distributions for both the isotropic and anisotropic damage models are presented in Figures 6.19-6.22.

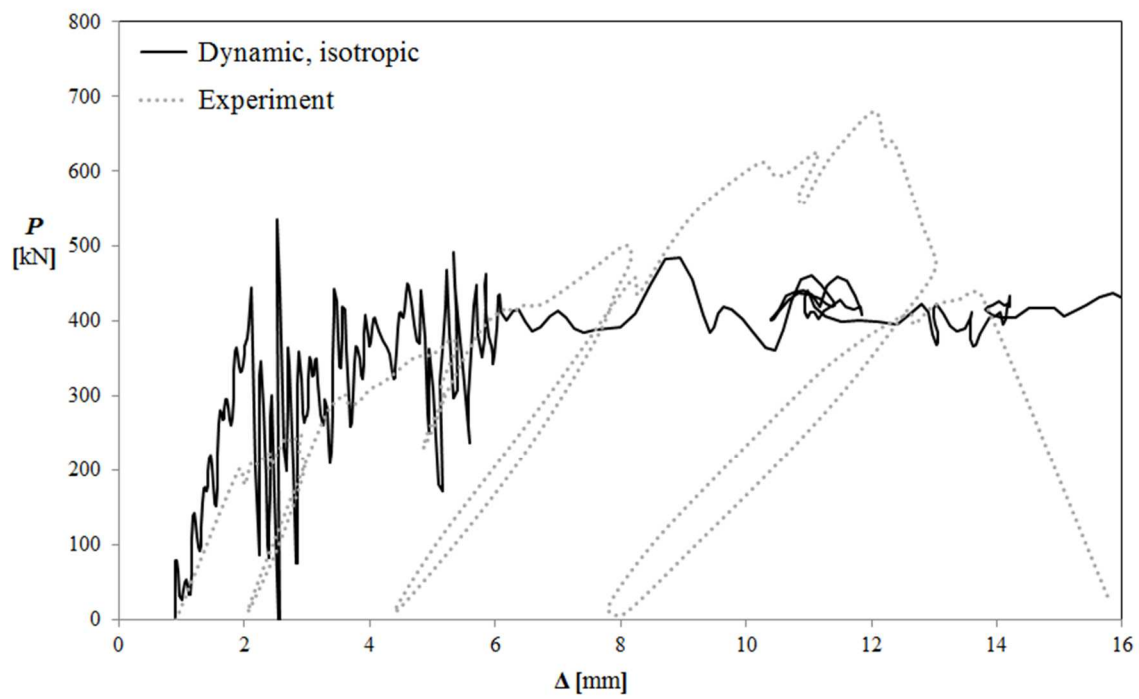
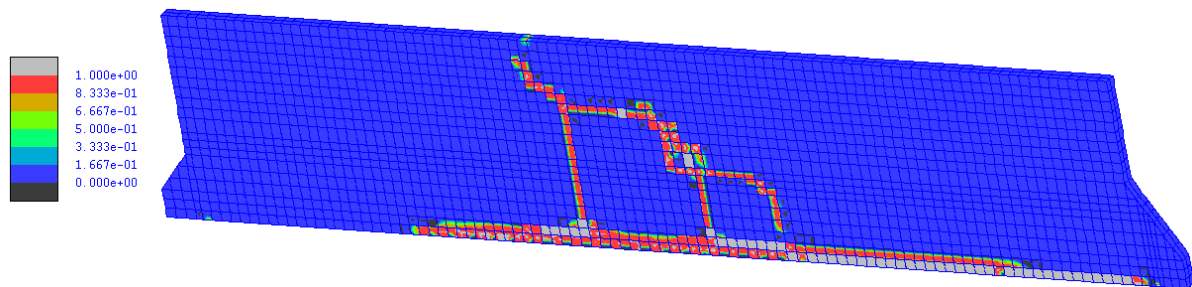


Figure 6.19: Dynamic response curve with isotropic damage

Figure 6.20: Scalar damage distribution under isotropic dynamic analysis ( $\Delta \approx 15.0$  mm)

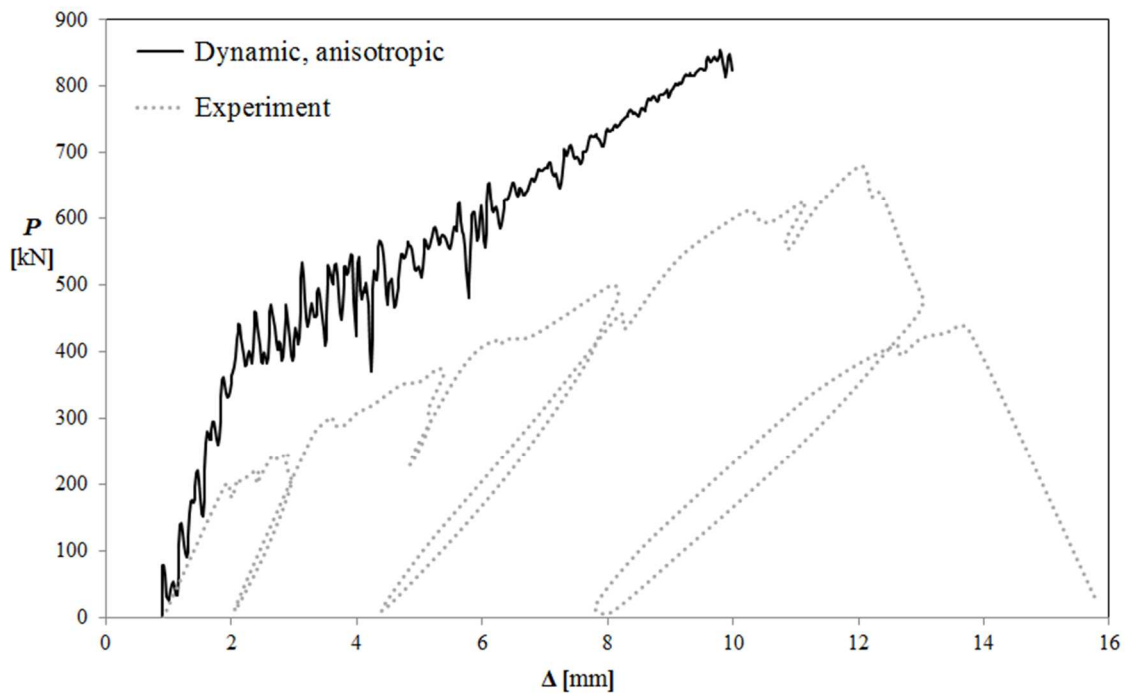


Figure 6.21: Dynamic response curve with anisotropic damage

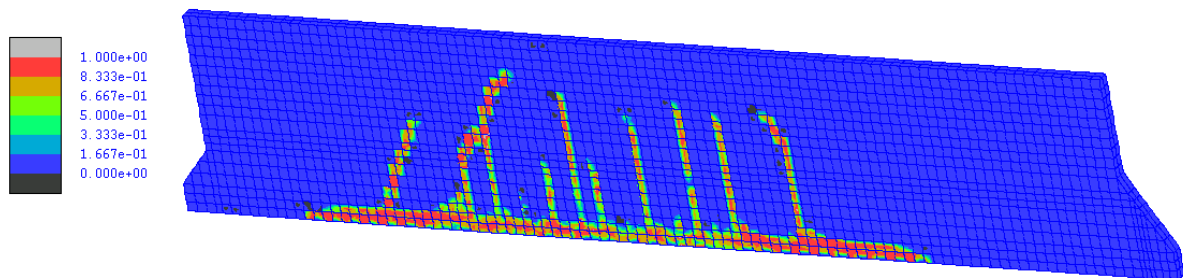


Figure 6.22: First principal damage component distribution under anisotropic dynamic analysis ( $\Delta \approx 10.0$  mm)

The isotropic damage response of the dynamic model is more prone to instabilities, particularly in the initial stage following onset of macro-cracking, where the snap-back under static analysis would occur. This eventually leads to a failure mode where the bottom horizontal layers mostly lose integrity due to extensive damage, despite the overlaying of elastic elements of residual stiffness. This artificial ‘splitting’ failure mode evolves alongside a diagonal crack before the observed peak load can be reached and explains the loss of stability observed in the response curve of Figure 6.19 from a certain displacement threshold onwards ( $\Delta \approx 6.5$  mm). On the other hand, the anisotropic damage response is capable of

progressing without great distortion induced by dynamic effects up to a load level of approximately 20% over the experimental failure load. The resulting damage distribution (Figure 6.22) shows that the main crack pattern in the west span is correctly reproduced, although the primary cracks in the east span fail to coalesce into the diagonal crack accompanying the observed failure. Such inability to capture the critical shear crack is considered to undermine this analysis, since the west span is expected to be much stronger than the east due to the combined effect of direct strutting action and shear reinforcement. When comparing the damage distribution of both damage models with the observed crack pattern, as shown in Figure 6.23, the main salient feature is the crossed correspondence of spans with these models. Anisotropic damage captures well the main cracks of the west span while isotropic damage only manages to reflect the main diagonal crack connecting with the ‘splitting’ cracks of the bottom layers. The underlying reason for this is unclear. On the one hand, the anisotropic damage model is not completely free of potential stress locking. Hence, in the presence of a misalignment between the crack or damage band and the mesh line orientation, the spurious shear stress transfer may lead to a greater mesh induced directional bias. This could explain the inability of the east span main cracks to curve and form the final diagonal crack. On the other hand, however, the tendency of the anisotropic damage model to a stiffer response, though potentially spurious in nature, should lead to a less developed crack pattern for a similar level of displacement. The fact that the isotropic model allows for the formation of the diagonal crack before the onset of macro-cracking in the west span constitutes a mismatch with this reasoning.

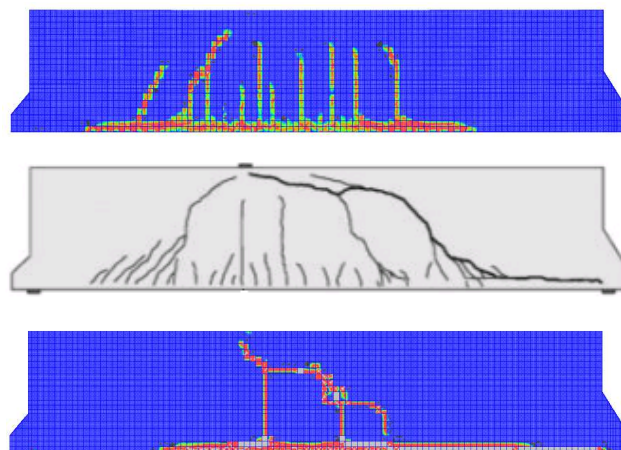


Figure 6.23: Observed crack pattern vs. anisotropic damage distribution (top) and isotropic damage distribution (bottom)

### 6.2.5 Conclusions

The large dimensions of the specimen pose a challenge from the numerical perspective, as material homogeneity in such an extensive domain leads to abrupt releases of energy upon formation of large cracks. These translate into instabilities in the response curve, in the form of successive snap-backs for which indirect displacement control is the only strategy facilitating the progress of the iterative procedure. It is believed that a sufficient number of indirect displacement control stages, linked to the appropriate nodes along the developed damage bands, will enable the tracking up to peak load and further to the softening branch. The reason for the discrepancy with the response curve of Červenka *et al.* (2016) cannot be fully established. As elaborated upon in previous chapters, the CDPM as implemented in this work resorts to a fully consistent tangential algorithmic stiffness that is retrieved at global level for the application of a full Newton-Raphson scheme. Shifting from a tangential to a secant approach may be the reason for the different curve trends after cracking, the latter not being able to trace the nonlinear equilibrium path as accurately (as a snap-back seems more consistent than a progressive decay with the fracture vs. strain energy balance in such a voluminous body) but indirectly benefitting from a larger step size under displacement control.

Resorting to a probabilistic description of the fracture energy and the tensile strength reflects more accurately the scatter in material properties of the real specimen and plays a significant role in the initiation of localisation. The coalescing into large damage bands becomes more gradual and this in turn reduces the magnitude of the snap-backs or unloading drops, as the energy upon cracking is released less abruptly.

The mixture of a region with reinforcement and distributed damage (bottom layers) and a mainly unreinforced region with large localised damage bands (middle third of the bulk between top and bottom reinforcement) is also of interest. As commented in Chapter 5, and following Rots (1988), the tendency to diffusion associated with perfect bond entails an apparent increase in the specific fracture energy. If the characteristic element size is kept as a fixed parameter, this in turn implies an apparent increase in fracture energy. Since the distributed damage band at the bottom layer propagates during the whole loading process

until effectively becoming a debonding crack, this effect may be of relevance in this case, magnifying the difficulties of the equilibrium tracking procedure to advance further.

A greater value of apparent fracture energy stemming from the distributed damage zone in the bottom layers could explain the good agreement between damage distribution and observed crack pattern for an assumed fracture energy parameter in the range  $\{5G_f^0, 10G_f^0\}$ , as well as the rough correspondence between rescaled response curves and the experimental curve in terms of dissipated energy. This reasoning is in line with the conclusions of Rots (1988) regarding the size-effect observed in concrete structures, leading to an increase of brittleness with the specimen dimensions. If the strain energy stored in the material increases alongside the size of the specimen in a greater rate than the fracture energy required to create a crack across it, then the global response would tend to be more abrupt, consistently with the snap-backs of the simulation and the tendency to a smoother evolution with increasing  $G_f$ . In terms of energy balance, however, this poses the question of the sensitivity of the response to the elastic and plastic parameters affecting the strain energy. Similar to the probabilistic approach to the distribution of  $\bar{f}_t$  and  $G_f$ , consideration of the spatial scatter of the main remaining parameters is expected to have an effect on the response.

Although the governing system of simultaneous equations loses ellipticity shortly after onset of damage, the significant slowdown in damage evolution following an increase in fracture energy appears to have an alleviating effect on mesh induced directional bias. This suggests a quantitative nature in the evolution of such effect, although further investigation would be required to assess this.

Under dynamic analysis, it is possible to track the response curve for greater displacement values than under static analysis. However, the dynamic isotropic damage model seems to be more sensitive to the ‘splitting’ failure mode of the bottom layers once they reach extensive damage states. The ensuing instabilities prevent the response to evolve further. The dynamic anisotropic model does reach a peak load, overestimating the experimental value by approximately 20%, although it is shown that stress locking is the potential source behind the overall stiffer response. Further reviewing is needed to evaluate these observations, as the damage distributions of the different damage models on both spans do not sustain this consistently.

It remains an open question to what extent the inclusion of bond slip would affect the outcome, as it facilitates the formation of primary cracks across reinforcement bars, hence opposing the tendency to distributed damage.

## 6.3 Case 2

The second case study refers to an experimental programme carried out in the École Polytechnique Fédérale de Lausanne and reported by Lips *et al.* (2012), focused on investigating the influence of certain geometric parameters and reinforcement arrangements on the punching shear strength and deformation capacity of slabs. In particular, the tests aimed at gaining further insight into the types of failure less present in the literature, i.e. failure occurring within the shear reinforced area or close to the column by crushing of the concrete struts.

### 6.3.1 Geometric description and test setup

The overall experimental programme comprises a complete set of 16 square (3 x 3 m) flat slabs on an internal column, as depicted in Figure 6.24.

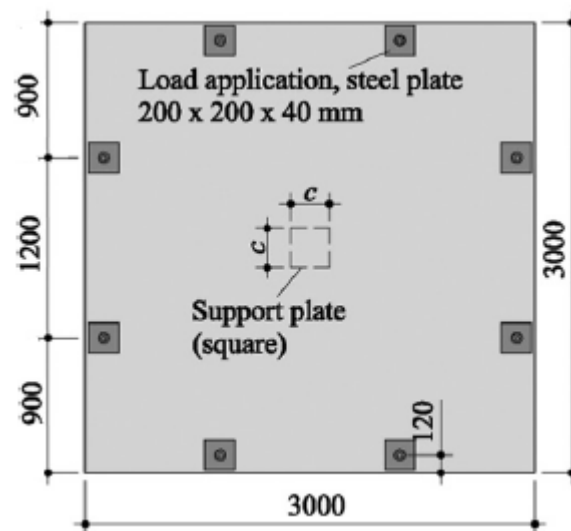


Figure 6.24: Geometry of test specimens (Lips *et al.*, 2012). Dimensions in mm.

The main varying parameters are the slab thickness ( $th$ ), the side length of the internal column ( $c$ ) and the adopted system of shear reinforcement. In the present work only a subset of slabs is considered for simulation, focusing on a single system of shear reinforcement, with the geometric and mechanical properties summarised in Table 6.1, whereby the original specimen nomenclature as per Lips *et al.* (2012) has been maintained.

| Specimen | [mm]<br>$th$ | [mm]<br>$c$ | [mm]<br>$d$ | System   | %<br>$\rho$ | %<br>$\rho_t$ |
|----------|--------------|-------------|-------------|----------|-------------|---------------|
| PL1      | 250          | 130         | 193         | —        | 1.63        | —             |
| PF1      | 250          | 130         | 209         | Stirrups | 1.50        | 0.79          |
| PL5      | 400          | 440         | 353         | —        | 1.50        | —             |
| PF5      | 400          | 440         | 354         | Stirrups | 1.50        | 0.79          |

Table 6.1: Main parameters of test specimens

In Table 6.1,  $d$  signifies effective depth and  $(\rho, \rho_t)$  stand for flexural and shear reinforcement ratio, respectively. The shear reinforcement system investigated comprises cages of continuous stirrups, which stem from bent bars welded together with straight 6 mm diameter bars. The system is schematically represented in Figure 6.25.

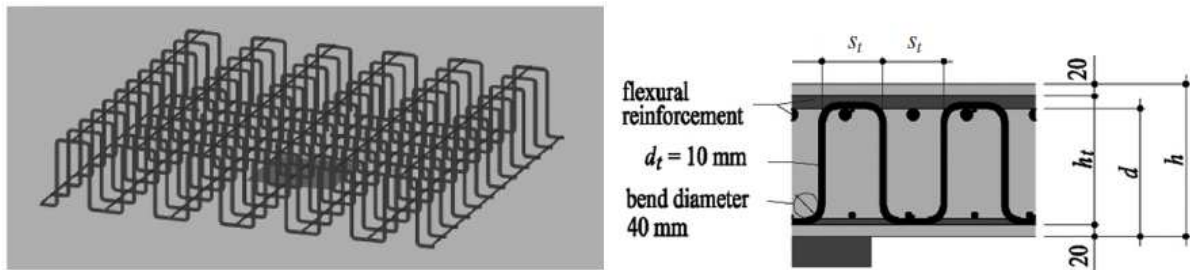


Figure 6.25: Punching shear reinforcement system: stirrup cages, adapted from Lips *et al.* (2012). Dimensions in mm.

The main geometric parameters of the shear reinforcement system are summarised in Table 6.2 and illustratively shown in Figure 6.26.

| Specimen | [mm]<br>$d_t$ | [mm]<br>$s_t$ | [mm]<br>$h_t$ | [mm]<br>$d_{TOP}$ | [mm]<br>$d_{BOT}$ |
|----------|---------------|---------------|---------------|-------------------|-------------------|
| PL1      | —             | —             | —             | 20                | 10                |
| PF1      | 10            | 100           | 200           | 20                | 10                |
| PL5      | —             | —             | —             | 26                | 10                |
| PF5      | 10            | 100           | 345           | 26                | 10                |

Table 6.2: Main parameters of shear and longitudinal reinforcement

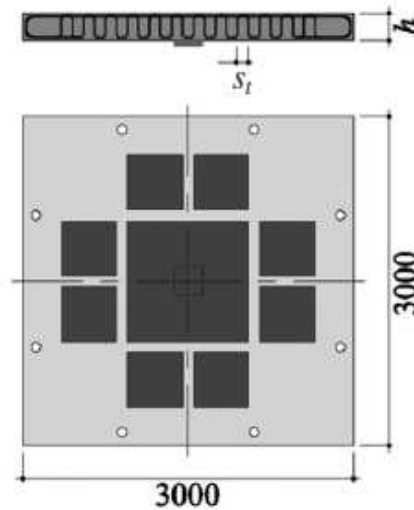


Figure 6.26: Punching shear reinforcement arrangement, adapted from Lips *et al.* (2012).

Dimensions in mm.

In Figures 6.25-6.26, as well as in Table 6.2,  $d_t$  stands for the diameter of the bent bar,  $s_t$  is the spacing between vertical branches of a stirrup and  $h_t$  is the height of the bent bar. A longitudinal reinforcement grid is provided at the top and bottom of each slab (Figure 6.25), with the corresponding diameters  $d_{TOP}$  and  $d_{BOT}$  as summarised in Table 6.2.

The vertical load is applied on the slab surface via eight steel plates symmetrically distributed (Figure 6.24). These constitute the last load transferring element of a system where the force is induced by hydraulic jacks and transmitted by means of tension bars and spreader beams. Further details regarding the test setup, materials and measurements can be found in Lips *et al.* (2012).

### 6.3.2 Mesh definition and parameters

For every slab, only the compressive strength of concrete ( $f_c$ ), the maximum aggregate size (16 mm) as well as the yield strength of all reinforcement elements ( $f_y, f_{yt}$ ) are provided in the original report. The remaining necessary parameters are estimated according to these given values, following the guidelines of CEB-FIP Model Code (1990), and are concisely collected in Table 6.3.

| Specimen | [MPa]<br>$f_c$ | [MPa]<br>$f_y$ | [MPa]<br>$f_{yt}$ | [GPa]<br>$E_c$ | [-]<br>$\nu$ | [MPa]<br>$f_t$ | [J/m <sup>2</sup> ]<br>$G_f$ | [GPa]<br>$E_s$ | [GPa]<br>$H$ |
|----------|----------------|----------------|-------------------|----------------|--------------|----------------|------------------------------|----------------|--------------|
| PL1      | 36.2           | 583            | —                 | 33.012         | 0.2          | 2.79           | 74                           | 200            | 0.02         |
| PF1      | 31.1           | 583            | 536               | 31.383         | 0.2          | 2.45           | 67                           | 200            | 0.02         |
| PL5      | 31.9           | 580            | —                 | 31.650         | 0.2          | 2.50           | 68                           | 200            | 0.02         |
| PF5      | 33.4           | 580            | 550               | 32.168         | 0.2          | 2.60           | 70                           | 200            | 0.02         |

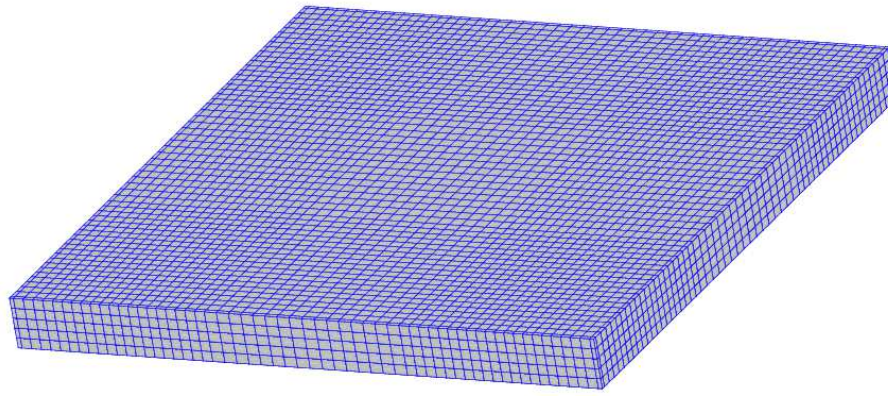
Table 6.3: Material parameters for all slab specimens

The yield strength values  $(f_y, f_{yt})$  refer to the flexural steel and shear reinforcement, respectively. Initially, the characteristic element size parameter is taken as  $h = 35$  mm for all meshes, as all of them maintain a similar degree of regularity and such value represents a minimum of 0.7 with respect to the average element size. Quadratic hexahedral elements are used to model the concrete bulk; their number in each mesh, along with the number of macro-segments representing the reinforcement, is shown in Table 6.4.

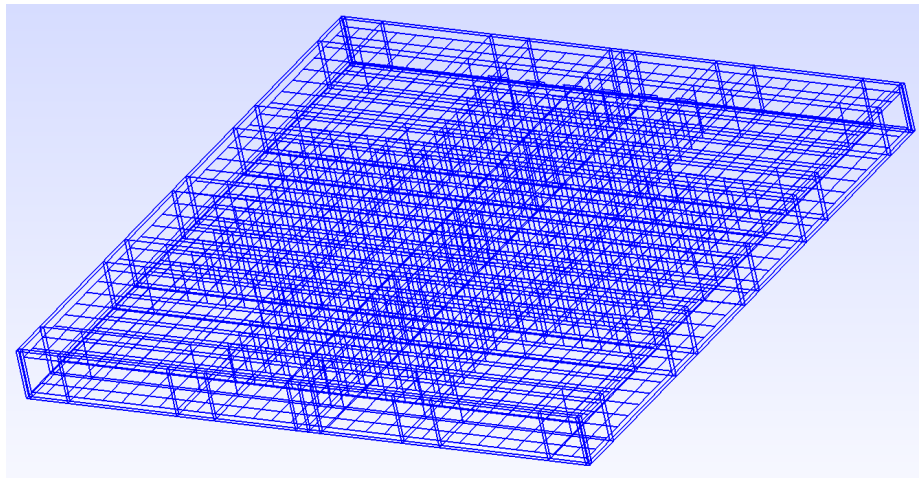
| Specimen | Concrete elements | Bar elements |
|----------|-------------------|--------------|
| PL1      | 16820             | 124          |
| PF1      | 16820             | 1492         |
| PL5      | 26912             | 124          |
| PF5      | 26912             | 1492         |

Table 6.4: Number of concrete and bar elements for all slab specimens

When discretising the reinforcement, longitudinal bars constitute entire bar elements themselves, whereas bent bars consist of a succession of vertical and horizontal bar elements connected by a common node, i.e. the bend diameter of Figure 6.25 is simplified to a sharp right angle corner. Illustratively, the concrete mesh of slab PL1 along with the bar mesh of slab PF1 are shown in Figure 6.27.



(a)



(b)

Figure 6.27: 250 mm thick slabs (a) PL1 concrete mesh (b) PF1 bar mesh

### 6.3.3 Static analysis

All nodes pertaining to the square area of the column head at the centre of the bottom face of the slabs are fully restrained, and the uniform loading of the steel plates is distributed as equivalent nodal forces, leading an initial load control stage. Subsequently, an arc-length control strategy guides the analysis to completion. Following the original report by Lips *et al.* (2012), the performance of all slabs is measured by means of load vs. rotation curves, as schematically shown in Figure 6.28. Measuring of rotation  $\psi$  is simplified to the ratio of average slab edge vertical displacement over a rotation arm, which is assumed as the clear distance from the support edge to the lateral end of the slab, reduced by half of the effective depth.

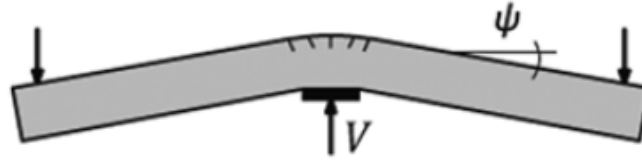


Figure 6.28: Load and rotation on a deformed slab (Lips *et al.*, 2012)

Figures 6.29-6.30 show the load vs. rotation response curves for the thinner slabs (PL1, PF1) and thicker slabs (PL5, PF5), respectively, along with the measured experimental results.

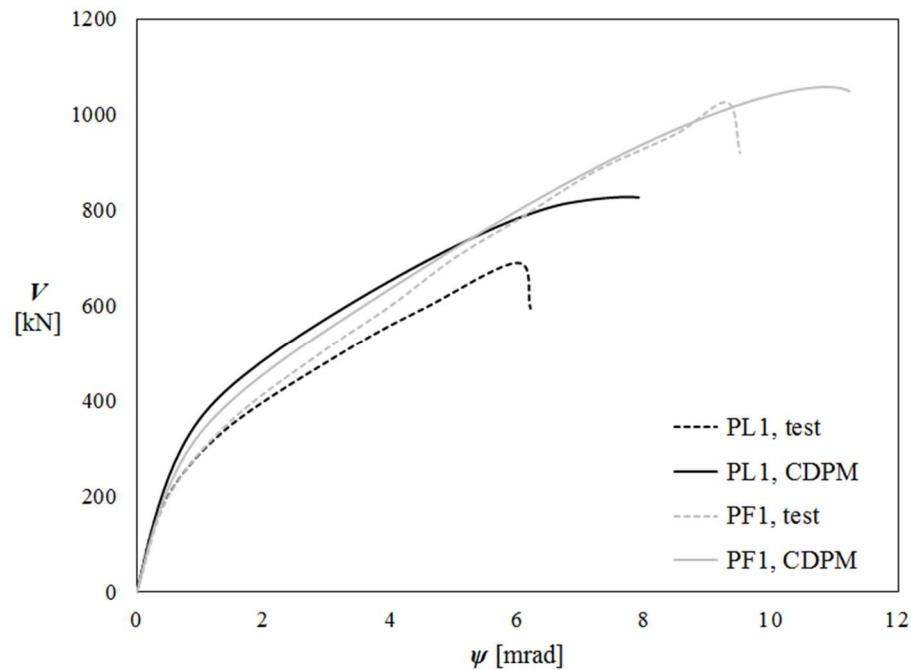


Figure 6.29: Load vs. rotation curve for slabs PL1 and PF1

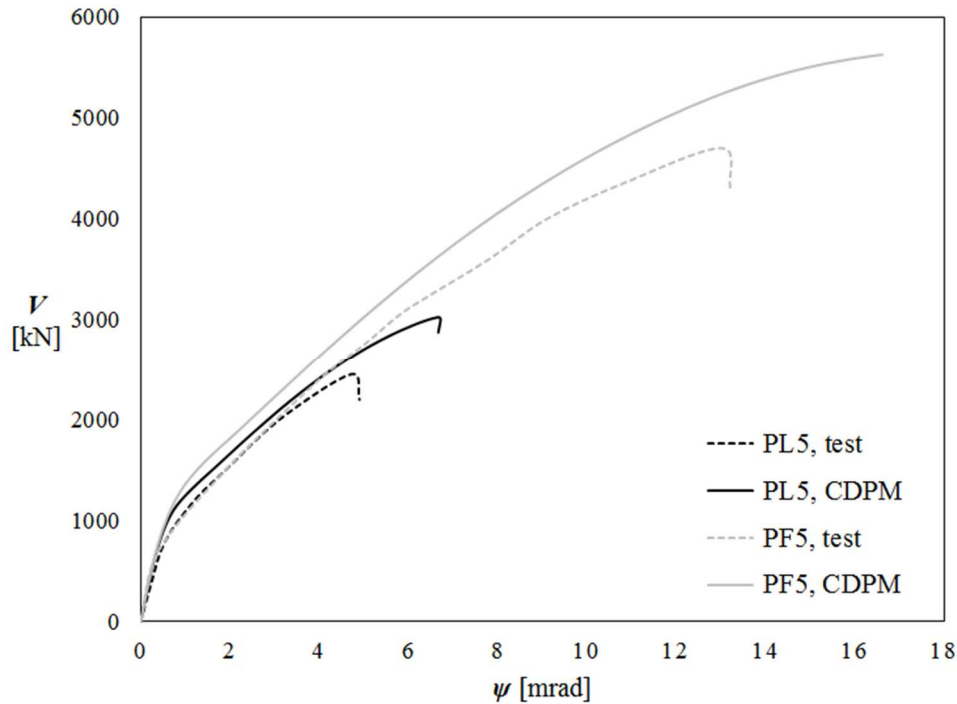


Figure 6.30: Load vs. rotation curve for slabs PL5 and PF5

In all cases, the equilibrium path could be traced up to peak load and beyond to commencement of softening. For the thinner slabs, symmetry is maintained in the east-west direction whereas along the north-south direction loss of symmetry is noticeable from early stages of cracking, as depicted in Figure 6.31 for slab PL1 at peak load (whereby a magnification factor of 20 is applied). For the thicker slabs, on the contrary, loss of symmetry becomes manifest along the north-south axis at later stages, considerably closer to peak load, as shown in Figure 6.32 for slab PL5. These asymmetries relate to imperfections, although the sources of such imperfections are unclear, as the PL slabs contain no shear reinforcement and, following the effective depth values of Table 6.2, the flexural reinforcement is assumed to lie on the same plane in both directions.

Table 6.5 summarises the numerical peak load values and associated rotations for all slabs, along with the reported test results. For both thickness values, the prediction error is of lesser magnitude in the case of slab with shear reinforcement. In particular, slab PF1 predicts the peak load value within 1.5%, and rotation within 15.0%. Simulations of slabs PL give rise to a more ductile response at peak, with overestimations of load of about 21%, although during hardening the evolution of rotations tends to be stiffer, especially for slab PL1.

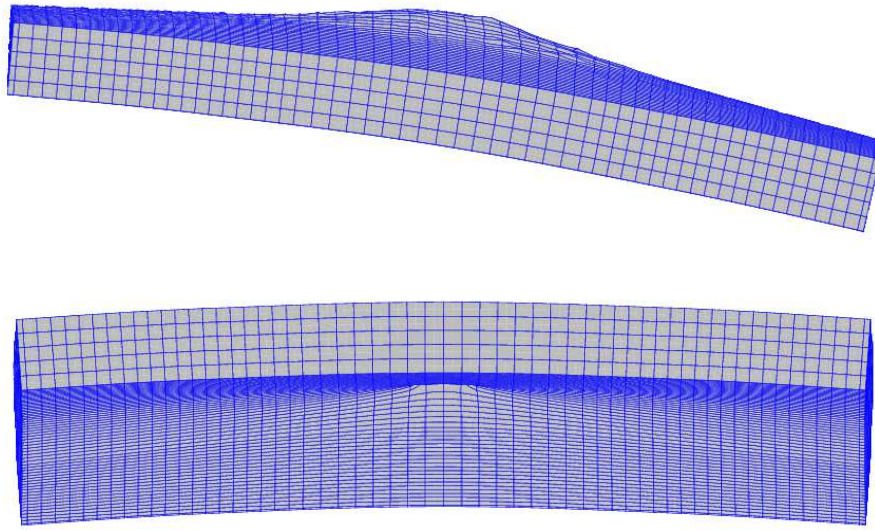


Figure 6.31: Slab PL1 at  $V_{\max}$  (top) north-south axis (bottom) east-west axis

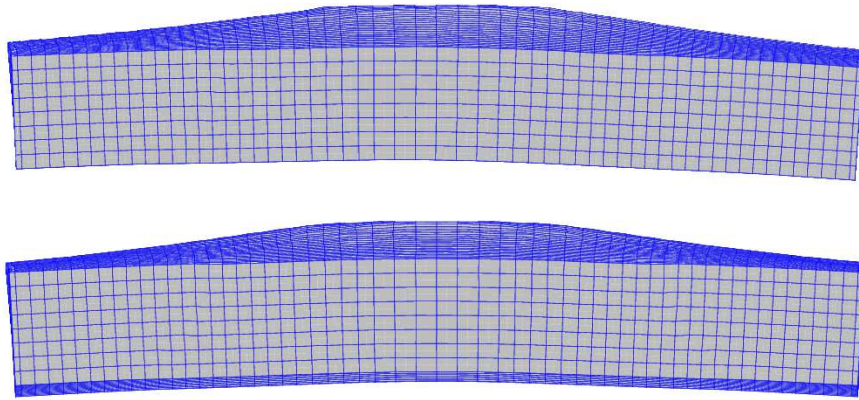


Figure 6.32: Slab PL5 at  $V_{\max}$  (top) north-south axis (bottom) east-west axis

| Specimen | [kN]       | [mrad] | [kN]              | [mrad]        |
|----------|------------|--------|-------------------|---------------|
|          | $V_{\max}$ | $\psi$ | $V_{\max}^{test}$ | $\psi_{test}$ |
| PL1      | 827        | 7.7    | 682               | 6.0           |
| PF1      | 1057       | 10.9   | 1043              | 9.5           |
| PL5      | 3024       | 6.6    | 2491              | 4.7           |
| PF5      | 5383       | 14.0   | 4717              | 13.4          |

Table 6.5: Reported and simulated load peak values and rotations

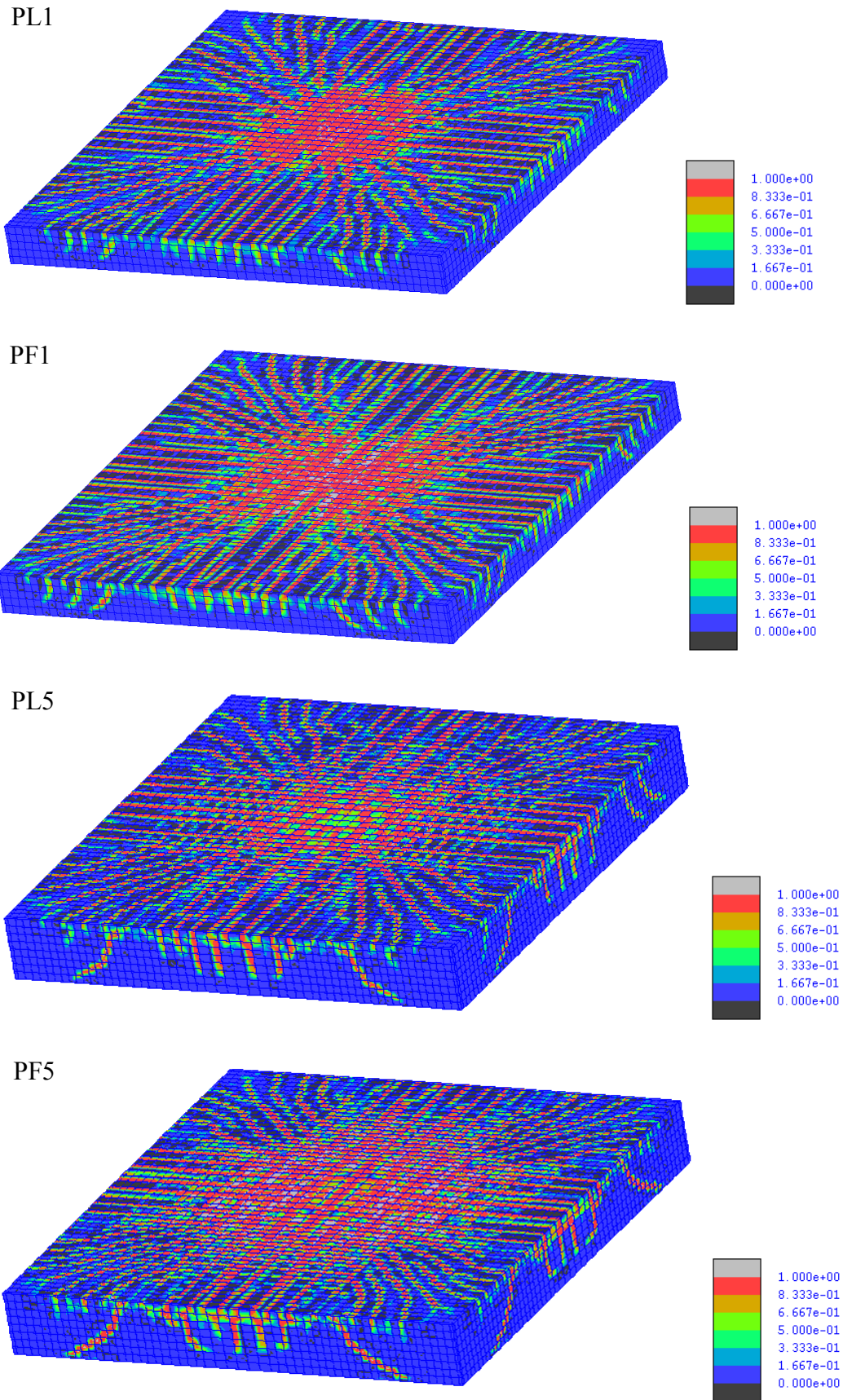
Figure 6.33: Damage variable  $\omega$  distribution of slabs at  $V_{\max}$

Figure 6.33 shows the scalar damage distributions for all slabs at peak load, which are consistent with a punching shear failure mode, although still subject to mesh-induced directional bias to a certain extent. The north-south and east-west mesh orientations are strongly influencing the evolution of the radial damage bands.

Furthermore, the resulting area of distributed damage above the column head poses the question of the choice of the fixed characteristic element size parameter  $h$ . Under such conditions, the notion of bandwidth is not intuitive to measure, as damage tends to shift from localised to diffuse. A greater value of  $h$  could result in more accurate predictions, although the fracture energy  $G_f$  would have to be reassessed as well. Recalling the argumentation of the first case study based on Rots (1988), transition to diffuse damage/cracking would entail an apparent increase in specific fracture energy ( $G_f/h$ ), which could explain why the PL slabs seem to require greater values of  $h$ . Hence, a sensitivity study of the response on  $h$  could help increasing the accuracy of slabs PL1, PL5 and PF5. This initiative, however, is not pursued further here.

Figure 6.34 shows a cut section of the slabs along the axis maintaining symmetry (east-west), where the distribution of scalar damage from Figure 6.33 across the cross-section is displayed, along with a comparison with the observed crack patterns after failure. Generally speaking, the damage distributions comply with the notion of failure occurring within the shear reinforced area towards the column head for PF slabs. However, coalescing into diagonal shear cracks is not properly captured, especially for PL slabs where these are less steep and more localised. Whilst damage distributes within the region of the column head in the thinner slabs, in the thick slabs damage propagates almost uniformly along the shear reinforcement area, only to partially coalesce close to the column faces.

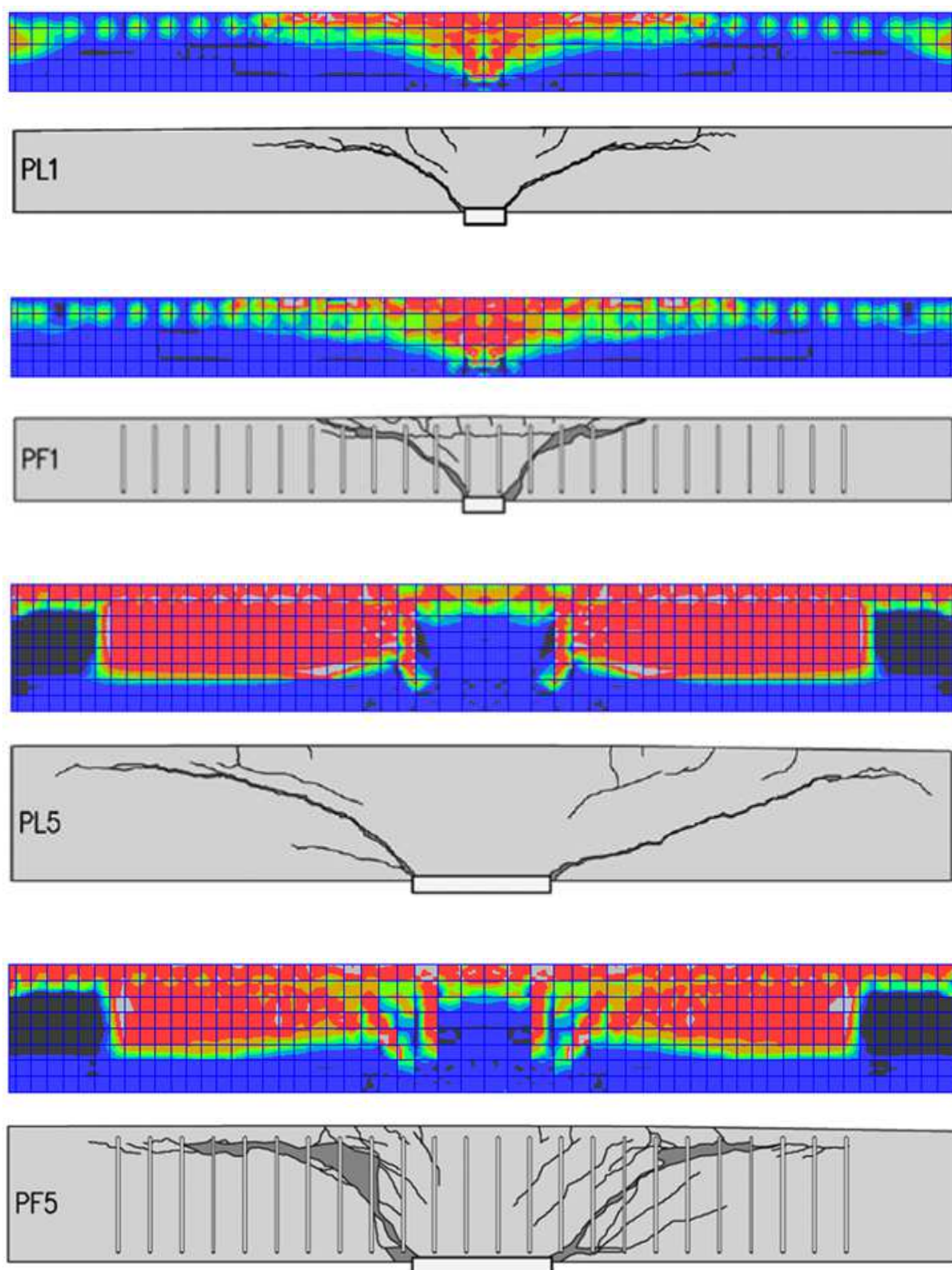


Figure 6.34: Comparison of damage distributions with experimental crack patterns  
(Lips *et al.*, 2012)

In Lips *et al.* (2012) it is argued that an indirect way of measuring the opening of the critical shear crack (Fernández Ruiz and Muttoni, 2009) is by means of measuring the change in slab thickness. To this end, a linear variable displacement transducer (LVDT), fixed to a rod traversing the slab through a hole (Figure 6.35), was used to track such variations in thickness.

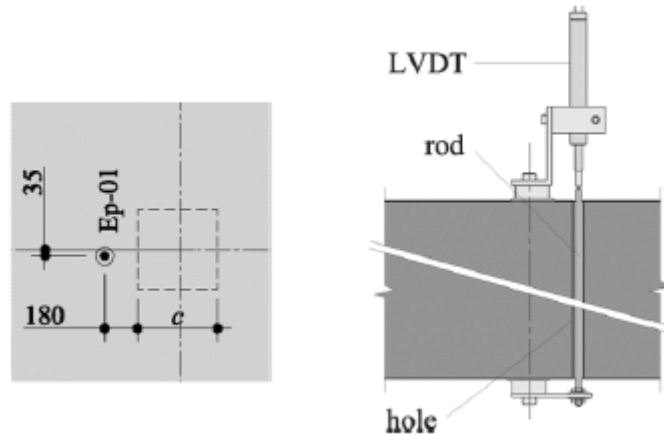


Figure 6.35: Location and arrangement of the LVDT to measure slab thickness  
(Lips *et al.*, 2012)

Figure 6.36 compares the measured and simulated variation in slab thickness during the loading process. Interestingly, in the simulations the change in thickness is initiated alongside the loading process, before any noticeable variations are recorded by the LVDT. Upon cracking, the expected relative variation in slab PL5 thickness with respect to slab PF5 does not occur, with both slabs thicknesses evolving equally until slab PL5 attains its strength value. The relative slowdown in slab thickness variation of slab PF5 is meant to represent the restraining effect of shear reinforcement on the opening of the critical shear crack. The coincidence of curves for both slabs in Figure 6.36 indicates that this effect cannot be captured and might explain the lack of coalescence in the damage distribution of slab PL5.

### 6.3.4 Conclusions

The loading process of all slab specimens is successfully simulated up to peak load, with the accuracy of load and rotation predictions being scattered over a wide range, from 1.5% for slab PF1 (load) to 40% for slab PL5 (rotation). It is suggested that PL slabs require a greater value of characteristic element size  $h$ , assumed identical for all cases, as the tendency from localised to diffuse damage has an augmentative effect on specific fracture energy, attaining

an apparent greater value. A sensitivity study on parameter  $h$  could indicate its optimal range, less intuitive when damage evolves in a distributed mode.

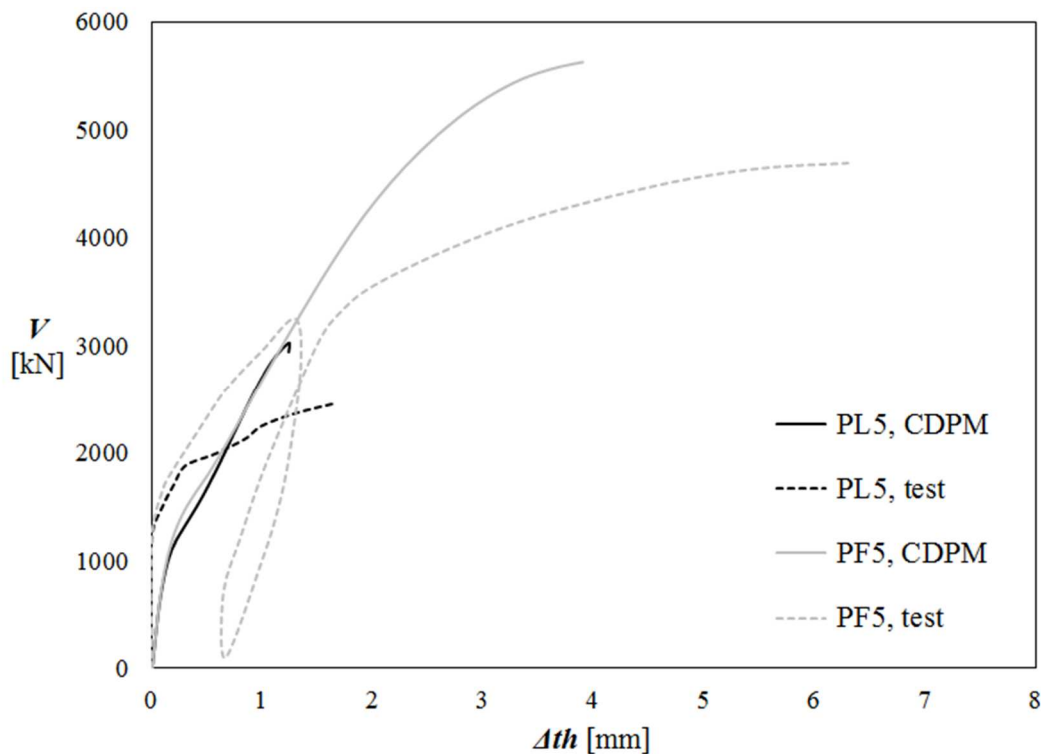


Figure 6.36: Variation in slab thickness from test measurements and numerical simulations

Symmetry of the failure mode is preserved along the east-west axis but not along the north-south axis. This asymmetry is associated with imperfections stemming from the concrete or the flexural reinforcement definitions.

Damage distributions tend to shift from a localised to a more diffuse shape, although overall concentrate in the column head or the shear reinforcement area as per the observed crack pattern and also comply with the form of a punching shear failure mode. It remains an open question to what extent would bond slip alleviate this shift. The lack of coalescing into a critical shear crack is further illustrated by tracking the variations in slab thickness, whereby the slab without shear reinforcement displays the same thickness variation rate as the slab with stirrup cages.

# CHAPTER 7

## Conclusions

### 7.1 Summary

Within the recent stream of high-fidelity modelling, which aims for an accurate representation of the true spatial material response of concrete, the work presented here focuses on a robust and efficient material model algorithm for three-dimensional analysis. This model is set at the macro-scale and within the framework of a smeared softening continuum formulation, consisting of a combination of plasticity and scalar damage. Following the choice of model, several challenges of numerical nature arise when evaluating the sources of decay in robustness, convergence or convergence rate. This research proposes algorithmic enhancements at material level for concrete, as well as at geometric level for the discretisation of embedded reinforcement bars. The application of these enhancements paves the way for an efficient three-dimensional modelling of reinforced concrete structures and contributes to the high fidelity description of complex substructures when resorting to dimensional coupling.

In the following sections, the principal conclusions arising from the main chapters of this thesis are concisely collected.

### 7.1.1 Algorithmic enhancements of the CDPM

The CDPM is chosen in this work as the reference material model for concrete, whereby focus is centred on its algorithmic structure and implementation strategy. Novel enhancements are introduced, involving the subdivision of the effective stress space to trigger different types of stress-returns, alongside a sequence of *a priori* and *a posteriori* checks and a line search scheme. These enhancements prove to significantly contribute to the numerical robustness of the implemented model.

The underlying reason for previous robustness issues is shown to be the potential singularity of the Jacobian at either the initial trial stress state or an intermediate iterative stress state. Whilst a reduction of the rank of simultaneous equations by decoupling the internal strain-like plastic variable proves thoroughly advantageous in the former case, the latter necessitates the proposed line search scheme to avoid Jacobian singularity or even convergence to inadmissible stress states.

Upon numerical testing of the implemented module, the increase in robustness is confirmed by achieving a full convergence ratio, which previous works fail to attain. The proposed modification to reconcile the discontinuity of returned stress states close to or strictly on the hydrostatic axis, though consistent and more intuitive, implies a decrease in the convergence rate for the numerical test, retaining full convergence ratio nonetheless, and is therefore discarded.

New provisions are presented whilst elaborating the elasto-plastic-damage algorithmic stiffness, in order to accommodate the case of stress-returns along the tensile or compressive meridian planes, hitherto untreated. The resulting consistent derivation of this operator enables the use of a full Newton scheme for the global boundary value problem upon implementation of the material model in the nonlinear Finite Element software ADAPTIC (Izzuddin, 1991).

By means of localisation analysis on the CDPM, the good directional properties of the model are confirmed, and its efficiency and robustness are corroborated by the results of a single element test, achieved despite the invariance of Lode's angle during stress return and a constant eccentricity parameter.

The original damage part of the CDPM is isotropic, and is extended in this work to anisotropic formulation, shifting the character of internal variable controlling the softening process to the trace of the damage tensor. Since damage is evaluated explicitly, this generalisation does not alter numerical robustness.

A suitable regularisation formulation via the crack band approach is reviewed and elaborated for the quadratic element types used in this work, although the computational convenience of a fixed damage bandwidth parameter is justified.

### **7.1.2 Algorithmic enhancements of the embedded bar model**

The embedded approach for modelling of reinforcement is selected as the most suitable, based on its capability of allowing arbitrary bar orientation within a concrete parent element. Hence, the concrete element mesh arrangement can be guided by stress considerations, effectively decoupled from the reinforcement arrangement.

The algorithm presented and discussed in this work incorporates additional novel features that allow for an efficient and robust treatment of discretised embedded bars, from their location within an arbitrary concrete mesh to their sequential tracking up to their end point. Embedded segments are not approximated by their chord and retain their interpolated shape. The described procedures are approached systematically and are readily applicable to any parent element type and geometry, accommodating every potential source of ambiguity in the form of bars lying on shared parent element faces, edges or vertex nodes, including the singular case of a pyramid apex. The resulting bar discretisation is shown to be accurate, without resorting to simplifications applied in previous models, and can sustain parent element distortions within the usual bounds to maintain unique relations between Cartesian and intrinsic coordinates.

The contribution of discretised embedded segments to their parent element stiffness matrix and nodal force vector is established, and the omission of an adjustment for the material overlap is justified. Implementation of these contributions along with the bar discretisation module into the nonlinear Finite Element software ADAPTIC (Izzuddin, 1991) allows for the simulation of reinforced concrete (monotonic) loading processes.

### 7.1.3 Numerical applications

The numerical examples presented and discussed in this work cover benchmark tests of different structural behaviour, and prove to constitute a reasonable framework in which to assess the validity of the enhanced concrete material model and the proposed embedded reinforcement approach.

The significant computational convenience of treating the characteristic element size  $h$  as a fixed parameter, as opposed to considering it a local internal variable based on a projection method, is confirmed with the notched three-point bending simulation. For more irregular mesh regions prone to contain a damage band, it would be preferable to define a finite set of values for  $h$  and externally distribute them based on mesh morphology considerations. In any case, although less systematic and sensitive to errors by the analyst, the benefits in performance justify the approach of fixing  $h$ .

Simulations of the torsion beam show that a convenient mesh morphology may alleviate the effects of mesh-induced directional bias. Hence, despite the loss of ellipticity at the global level and the consequent loss of solution uniqueness, it is still possible for the damage band to propagate in the correct direction provided that it pertains to the directions made available by the mesh main orientations. In any case, it is also shown that even biased solutions dissipate approximately the same amount of energy.

Applying localisation analysis to the CDPM does not contribute noticeably to overcome mesh-induced directional bias if the appropriate damage propagation direction is not facilitated by the mesh orientation. Furthermore, the need for tracking the potential singularity of the localisation tensor for each sample point severely hinders performance.

The extension of the CDPM to anisotropic damage does not noticeably alter the global response in terms of peak load prediction or damage distribution, although a minor increment in dissipated energy is noted for the same mesh type and characteristic element size.

Resorting to hierarchical partition modelling, particularly under dynamic analysis of the PCT-3D specimen, is shown to improve performance, allowing for a significantly larger output for the same computing time as a monolithic model. This confirms the capabilities of this

numerical technique, which is corroborated by the unnotched three-point bending reinforced concrete test simulation. Shifting from static to dynamic analysis, however, does not entail benefits regarding the mesh-induced directional bias.

The uniaxial compression test simulations for a cube and a cylinder corroborate the capability of the model to reflect damage propagation arising under compressive states. In these circumstances, however, particularly if damage tends to be diffuse, the choice of a fixed parameter representing a characteristic element size becomes less intuitive.

The reinforced concrete beam simulations highlight the importance of the fracture energy estimation, particularly for laboratory-size specimens. In its current form, the model seems to display a strong sensitivity to the presence of reinforcement bars with perfect bond, with a tendency to necessitate greater values of fracture energy than code estimations to dissipate energy correctly. This feature can be associated to the transition from localised to diffuse damage, a trend reinforced by the perfect bond assumption, but is not entirely consistent here.

#### **7.1.4 Major case studies**

The large dimensions of the specimen in the first case study pose a challenge from the numerical perspective, as material homogeneity in such an extensive domain leads to abrupt releases of energy upon formation of large cracks. These translate into instabilities in the response curve, in the form of successive snap-backs for which indirect displacement control is the only strategy facilitating the progress of the iterative procedure. It is believed that a sufficient number of indirect displacement control stages, linked to the appropriate nodes along the developed damage bands, will enable the tracking up to peak load and further to the softening branch. The reason for the discrepancy with the response curve of Červenka *et al.* (2016) cannot be fully established. As shown in this work, the implemented CDPM resorts to a fully consistent tangential algorithmic stiffness that is retrieved at global level for the application of a full Newton-Raphson scheme. Shifting from a tangential to a secant approach may be the reason for the different curve trends after cracking, the latter not being able to trace the nonlinear equilibrium path as accurately (as a snap-back seems more consistent than a progressive decay with the fracture vs. strain energy balance in such a voluminous body) but indirectly benefitting from a larger step size under displacement control.

Resorting to a probabilistic description of the fracture energy and the tensile strength reflects more accurately the scatter in material properties of the real specimen and plays a significant role in the initiation of localisation. The coalescing into large damage bands becomes more gradual and this in turn reduces the magnitude of the snap-backs or unloading drops, as the energy upon cracking is released less abruptly.

The mixture of a region with reinforcement and distributed damage (bottom layers) and a mainly unreinforced region with large localised damage bands (middle third of the bulk between top and bottom reinforcement) is also of interest. Following Rots (1988), the tendency to diffusion associated to perfect bond entails an apparent increase in the specific fracture energy. If the characteristic element size is kept as a fixed parameter, this in turn implies an apparent increase in fracture energy. Since the distributed damage band at the bottom layer propagates during the whole loading process until effectively becoming a debonding crack, this effect may be of relevance in this case, magnifying the difficulties of the equilibrium tracking procedure to advance further.

A greater value of apparent fracture energy stemming from the distributed damage zone in the bottom layers could explain the good agreement between damage distribution and observed crack pattern for an assumed fracture energy parameter in the range  $\{5G_f^0, 10G_f^0\}$ , as well as the rough correspondence between rescaled response curves and the experimental curve in terms of dissipated energy. This reasoning is in line with the conclusions of Rots (1988) regarding the size-effect observed in concrete structures, leading to an increase of brittleness with the specimen dimensions. If the strain energy stored in the material increases alongside the size of the specimen in a greater rate than the fracture energy required to create a crack across it, then the global response would tend to be more abrupt, consistently with the snap-backs of the simulation and the tendency to a smoother evolution with increasing  $G_f$ . In terms of energy balance, however, this poses the question of the sensitivity of the response to the elastic and plastic parameters affecting the strain energy. Similar to the probabilistic approach to the distribution of  $\bar{f}_t$  and  $G_f$ , consideration of the spatial scatter of the main remaining parameters is expected to have an effect on the response.

Although the governing system of simultaneous equations loses ellipticity shortly after onset of damage, the significant slowdown in damage evolution following an increase in fracture

energy appears to have an alleviating effect on mesh induced directional bias. This suggests a quantitative nature in the evolution of such effect, although further investigation would be required to assess this.

Under dynamic analysis, it is possible to track the response curve for greater displacement values than under static analysis. However, the dynamic isotropic damage model seems to be more sensitive to the ‘splitting’ failure mode of the bottom layers once they reach extensive damage states. The ensuing instabilities prevent the response to evolve further. The dynamic anisotropic model does reach a peak load, overestimating the experimental value by approximately 20%, although it is shown that stress locking is the potential source behind the overall stiffer response. Further reviewing is needed to evaluate this, as the damage distributions of the different damage models on both spans do not sustain this consistently.

It remains an open question to what extent the inclusion of bond slip would affect the outcome, as it facilitates the formation of primary cracks across reinforcement bars, hence opposing the tendency to distributed damage.

In the second case study, the loading process of all slab specimens is successfully simulated up to peak load, with the accuracy of load and rotation predictions being scattered over a wide range, from 1.5% for slab PF1 (load) to 40% for slab PL5 (rotation). It is suggested that PL slabs require a greater value of characteristic element size  $h$ , assumed identical for all cases, as the tendency from localised to diffuse damage has an augmentative effect on specific fracture energy, attaining an apparent greater value. A sensitivity study on parameter  $h$  could indicate its optimal range, less intuitive when damage evolves in a distributed mode.

Symmetry of the failure mode is only preserved along the east-west axis but not along the north-south axis. This asymmetry is associated with imperfections stemming from the concrete or the flexural reinforcement definitions.

Damage distributions tend to shift from a localised to a more diffuse shape, although overall concentrate in the column head or the shear reinforcement area as per the observed crack pattern and also comply with the form of a punching shear failure mode. It remains an open question to what extent would bond slip alleviate this shift. The lack of coalescing into a critical shear crack is further illustrated by tracking the variations in slab thickness, whereby

the slab without shear reinforcement displays the same thickness variation rate as the slab with stirrup cages.

## 7.2 Recommendations for future work

Although the enhanced material model for concrete has demonstrated its significant contributions to local robustness and global performance, there is room for further improvements towards a more comprehensive set of loading scenarios for reinforced concrete structures under high-fidelity modelling. Potential research extensions in this regard include:

- Consideration of cyclic loading. Owing to the single scalar parameter for isotropic damage, there is no separate memory for damage evolution under tensile and compressive states. Hence, the material model at its current state can only accommodate monotonic loading. In order to retain the benefits arising from the enhancements introduced in the plastic part of the model, modifications should be applied only to the damage definition. One interesting option would be to combine isotropic and anisotropic damage to account for compressive and tensile stress states, respectively, shifting from one to two strain-like internal variables to track separate equivalent strain histories. The associated algorithmic stiffness would be a combination of the expressions derived separately in this work, allowing for global quadratic convergence rate.
- Alternatively, the algorithmic enhancements developed in this work could be adapted to CDPM2 (Grassl *et al.* (2013)), bearing in mind the differences in the definition of the initial nonlinear plastic hardening and the residual linear hardening. The latter implies a continuously shifting yield surface in principal stress space, hence disabling the direct apex return and the advantages of a fixed Menétrey-Willam surface. Further enhancements would be necessary to ensure Jacobian regularity during residual linear hardening. A modification of the compressive damage law to a linear or bilinear shape would be the only way to ensure the explicit derivation of the algorithmic stiffness.
- Inclusion of non-mechanical strains. A further source of nonlinearity not considered in this work is due to creep or shrinkage, which could be included as an extra term in the decomposition of strains into elastic and plastic. Any potential model in this regard, however, should be consistent with the main aims of robustness and

performance, and be compatible with the enhancements affecting the plastic part of the model.

- Along the lines of Folino and Etse (2012), the geometry of the plastic yield function could be made dependent on an additional term (originally called performance parameter) to allow for a unified frame in which to model normal and high-strength concrete.

From the perspective of the embedded reinforcement algorithm, there are also interesting potential improvements to better reflect real reinforcement behaviour:

- Inclusion of bond slip and dowel action. Formally following the same steps describing the axial contribution of an embedded bar segment to its parent element stiffness and force vector, transversal degrees of freedom could also be accommodated. A bond slip definition would allow the formation of primary cracks across the bar, potentially facilitating the localised propagation of damage instead of distributed with dense reinforcement arrangements.
- Generalisation of the sequential linearisation procedure to include the tracking of curved bars (in Cartesian space). Although generalisation is not ensured for any arbitrary deformed bar shape, it is possible for the relevant cases of interest in engineering practice: circular arches connecting straight segments, which could accurately reflect the standard bar bending induced by the mandrel, and polynomial segments, common for the definition of prestress tendon profiles. In such cases, when advancing along a bar axis in Cartesian space during a given linearisation, the evaluation of the step length would not be explicit. Instead, integration of rational functions (with square roots of polynomials) would be required, which is feasible for the aforementioned cases.

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# APPENDIX A

## Algorithmic stiffness with sub-incrementation

If a sub-incrementation scheme is applied in the stress evaluation algorithm described in Chapter 3, the algorithmic elasto-plastic-damage stiffness must be adapted consistently to ensure that quadratic convergence rate is kept. To this end, the formal procedure elaborated in Valentini (2011) under full formulation, accounting for all Cartesian effective stress components and a set of internal variables and plastic multipliers arising from a multi-surface plasticity approach, is modified hereafter to comply with the provisions of this work. The radial stress-returns along fixed meridian planes and the proposed intuitive geometric treatment of the apexes allows for a much compact system of simultaneous equations (rank 4 in the most generic case).

Sub-incrementation, as adopted by Valentini (2011) from the method proposed by Pérez-Foguet *et al.* (2001), implies a further division of the total strain increment at a step  $(n+1)$  into  $m$  sub-increments:

$$\Delta \boldsymbol{\varepsilon}^{(n+1)} = \sum_{j=1}^m \Delta \boldsymbol{\varepsilon}^{(n+j/m)} = \sum_{j=1}^m \beta^{(n+j/m)} \Delta \boldsymbol{\varepsilon}^{(n+1)} \quad (\text{A.1})$$

with:

$$0 < \beta^{(n+j/m)} = \frac{\Delta \boldsymbol{\varepsilon}^{(n+j/m)}}{\Delta \boldsymbol{\varepsilon}^{(n+1)}} \leq 1 \quad (\text{A.2})$$

signifying the ratio between the cumulative strain sub-increment at substep  $j$  and the total strain increment. When integrating the rate form of the constitutive equations for a (pseudo)time sub-increment, the residual system of equations (Figure 3.2) transforms into:

$$\begin{aligned}
 \bar{\sigma}_V^{(n+j/m)} &= \bar{\sigma}_V^{tr,(n+j/m)} - K \Delta\lambda^{(n+j/m)} m_V^{(n+j/m)} \left( \bar{\sigma}^{(n+j/m)}, \kappa_p^{(n+j/m)} \right) \\
 \bar{\rho}^{(n+j/m)} &= \bar{\rho}^{tr,(n+j/m)} - 2G \Delta\lambda^{(n+j/m)} m_D^{(n+j/m)} \left( \bar{\sigma}^{(n+j/m)}, \kappa_p^{(n+j/m)} \right) \\
 \kappa_p^{(n+j/m)} &= \kappa_p^{(n+(j-1)/m)} + \Delta\lambda^{(n+j/m)} k_p^{(n+j/m)} \left( \bar{\sigma}^{(n+j/m)}, \kappa_p^{(n+j/m)} \right) \\
 f_p^{(n+j/m)} \left( \bar{\sigma}^{(n+j/m)}, \kappa_p^{(n+j/m)} \right) &= 0
 \end{aligned} \tag{A.3}$$

where the superscript for iteration  $k$  has been dropped for clarity, as the states of reference are the converged ones for each strain sub-increment. The associated Jacobian matrix  $\mathbf{Jac}_{(n+j/m)}$  retains the structure given in (1.78). Consistent linearisation for a given sub-increment  $j$  leads to:

$$\begin{Bmatrix} \delta\bar{\sigma}_V^{(n+j/m)} \\ \delta\bar{\rho}^{(n+j/m)} \\ \delta\kappa_p^{(n+j/m)} \\ \delta(\Delta\lambda^{(n+j/m)}) \end{Bmatrix} = \mathbf{Jac}_{(n+j/m)}^{-1} \cdot \begin{Bmatrix} \delta\bar{\sigma}_V^{(n+(j-1)/m)} + K\delta : \delta(\Delta\epsilon^{(n+j/m)}) \\ \delta\bar{\rho}^{(n+(j-1)/m)} + \frac{2G}{\bar{\rho}^{tr,(n+j/m)}} \mathbf{s}^{tr,(n+j/m)} : \delta(\Delta\epsilon^{(n+j/m)}) \\ \delta\kappa_p^{(n+(j-1)/m)} \\ - \left[ \left( \frac{\partial f_p}{\partial \theta} \right) \delta\bar{\theta}^{tr} \right]^{(n+(j-1)/m)} - \left[ \left( \frac{\partial f_p}{\partial \theta} \right) \delta\bar{\theta}^{tr} \right]^{(n+j/m)} \end{Bmatrix} \tag{A.4}$$

The sub-incremental tangential operators are defined as:

$$\mathbf{\Theta}_{EP}^{(n+j/m)} = \begin{bmatrix} \frac{\partial \bar{\sigma}_V^{(n+j/m)}}{\partial \epsilon^{(n+1)}} \\ \frac{\partial \bar{\rho}^{(n+j/m)}}{\partial \epsilon^{(n+1)}} \end{bmatrix} \tag{A.5}$$

$$\mathbf{Q}_{EP}^{(n+j/m)} = \begin{bmatrix} \frac{\partial \kappa_p^{(n+j/m)}}{\partial \epsilon^{(n+1)}} \end{bmatrix} \tag{A.6}$$

$$\mathbf{L}_{EP}^{(n+j/m)} = \begin{bmatrix} \frac{\partial (\Delta\lambda^{(n+j/m)})}{\partial \epsilon^{(n+1)}} \end{bmatrix} \tag{A.7}$$

and can be derived from (A.4) by resorting to projection matrices as per Ortiz and Martin (1989):

$$\mathbf{P}^\sigma = [\mathbf{I}_2 \quad \mathbf{0}_2 \quad \mathbf{0}_2]^T \tag{A.8}$$

$$\mathbf{P}^\kappa = [\mathbf{0}_2 \quad \mathbf{I}_1 \quad \mathbf{0}_1]^T \tag{A.9}$$

$$\mathbf{P}^\lambda = [\mathbf{0}_2 \quad \mathbf{0}_1 \quad \mathbf{I}_1]^T \tag{A.10}$$

with the subscript in the submatrices indicating the order of the unit or zero matrix component. Hence, application of (A.8)-(A.10) when substituting (A.4) in (A.5)-(A.7) leads to:

$$\begin{aligned} \Theta_{EP}^{(n+j/m)} &= (\mathbf{P}^\sigma)^T \mathbf{Jac}_{(n+j/m)}^{-1} \left[ \mathbf{P}^\sigma : \left( \Theta_{EP}^{(n+(j-1)/m)} + \beta^{(n+j/m)} \mathbf{C}^{(n+j/m)} \right) + \mathbf{P}^\kappa : \mathbf{Q}_{EP}^{(n+(j-1)/m)} \right] \\ &\quad - (\mathbf{P}^\sigma)^T \mathbf{Jac}_{(n+j/m)}^{-1} \left[ \mathbf{P}^\lambda : \left[ \left( \frac{\partial f_p}{\partial \theta} \Psi_{EP} \right)^{(n+(j-1)/m)} + \left( \frac{\partial f_p}{\partial \theta} \Psi_{EP} \right)^{(n+j/m)} \right] \right] \end{aligned} \quad (\text{A.11})$$

$$\begin{aligned} \mathbf{Q}_{EP}^{(n+j/m)} &= (\mathbf{P}^\kappa)^T \mathbf{Jac}_{(n+j/m)}^{-1} \left[ \mathbf{P}^\sigma : \left( \Theta_{EP}^{(n+(j-1)/m)} + \beta^{(n+j/m)} \mathbf{C}^{(n+j/m)} \right) + \mathbf{P}^\kappa : \mathbf{Q}_{EP}^{(n+(j-1)/m)} \right] \\ &\quad - (\mathbf{P}^\kappa)^T \mathbf{Jac}_{(n+j/m)}^{-1} \left[ \mathbf{P}^\lambda : \left[ \left( \frac{\partial f_p}{\partial \theta} \Psi_{EP} \right)^{(n+(j-1)/m)} + \left( \frac{\partial f_p}{\partial \theta} \Psi_{EP} \right)^{(n+j/m)} \right] \right] \end{aligned} \quad (\text{A.12})$$

$$\begin{aligned} \mathbf{L}_{EP}^{(n+j/m)} &= (\mathbf{P}^\lambda)^T \mathbf{Jac}_{(n+j/m)}^{-1} \left[ \mathbf{P}^\sigma : \left( \Theta_{EP}^{(n+(j-1)/m)} + \beta^{(n+j/m)} \mathbf{C}^{(n+j/m)} \right) + \mathbf{P}^\kappa : \mathbf{Q}_{EP}^{(n+(j-1)/m)} \right] \\ &\quad - (\mathbf{P}^\lambda)^T \mathbf{Jac}_{(n+j/m)}^{-1} \left[ \mathbf{P}^\lambda : \left[ \left( \frac{\partial f_p}{\partial \theta} \Psi_{EP} \right)^{(n+(j-1)/m)} + \left( \frac{\partial f_p}{\partial \theta} \Psi_{EP} \right)^{(n+j/m)} \right] \right] \end{aligned} \quad (\text{A.13})$$

where the following auxiliary entities are used in (A.11)-(A.13):

$$\mathbf{C}^{(n+j/m)} = \begin{bmatrix} K\delta \\ \frac{2G}{\bar{\rho}^{tr,(n+j/m)}} \mathbf{s}^{tr,(n+j/m)} \end{bmatrix} \quad (\text{A.14})$$

$$\Psi_{EP}^{(n+j/m)} = \frac{\partial \bar{\theta}^{(n+j/m)}}{\partial \boldsymbol{\varepsilon}^{(n+1)}} \quad (\text{A.15})$$

(A.15) can be obtained directly from (1.112) or (1.122). By noting that  $\Theta_{EP}^{(n+0/m)} = \mathbf{Q}_{EP}^{(n+0/m)} = \mathbf{0}$ , the elasto-plastic algorithmic stiffness  $\Theta_{EP}^{(n+1)}$  results from (A.11) by cumulative updates at the end of all sub-increments within a strain increment. In order to accommodate the damage perturbation within a sub-increment, (1.124) is treated analogously to the residual system of equations, leading to the following sub-incremental damage tangential operator:

$$\mathbf{W}^{(n+j/m)} = \frac{\partial \omega^{(n+j/m)}}{\partial \boldsymbol{\varepsilon}^{(n+1)}} = \mathbf{W}^{(n+(j-1)/m)} + \left[ W_1 \frac{\partial \bar{\sigma}_V^{(n+j/m)}}{\partial \boldsymbol{\varepsilon}^{(n+1)}} + W_2 \frac{\partial \bar{\rho}^{(n+j/m)}}{\partial \boldsymbol{\varepsilon}^{(n+1)}} + W_3 \frac{\partial \kappa_p^{(n+j/m)}}{\partial \boldsymbol{\varepsilon}^{(n+1)}} + W_4 \frac{\partial (\Delta \lambda^{(n+j/m)})}{\partial \boldsymbol{\varepsilon}^{(n+1)}} \right] \quad (\text{A.16})$$

Coefficients  $\mathcal{W}_{1..4}$  have been introduced in (A.16) for clarity and compactness purposes, and can be expanded by inspection of (1.124). Since all derivatives in (A.16) can be obtained by successive application of (A.11)-(A.13) along the whole sub-incremental sequence, the cumulative damage perturbation results directly from  $\mathcal{W}^{(n+1)}$ . Recalling (1.126), the sought expression for the algorithmic elasto-plastic-damage stiffness evaluated at the end of a sub-incremented step is finally given by:

$$\left(1 - \omega^{(n+1)}\right) \mathbf{\Theta}_{EP}^{(n+1)} - \bar{\boldsymbol{\sigma}}^{(n+1)} \otimes \mathcal{W}^{(n+1)} \quad (\text{A.17})$$

# APPENDIX B

## Supplementary terms of the algorithmic stiffness

The assumption of taking  $\mathbf{n}$  in (3.122) as the first strain eigenvector introduces a directional dependency of  $h$  on the spectral matrix as evaluated in the perturbed trial stress state. As a result of this dependency, an additional term arises in the derivation of the elasto-plastic-damage algorithmic stiffness, in particular in the term involving the perturbation of damage. For the scalar isotropic damage case, this perturbation is expressed as:

$$\delta\omega = \frac{\partial g_d}{\partial \kappa_d} \delta\tilde{\varepsilon} + \frac{\partial g_d}{\partial \varepsilon_f} \delta\varepsilon_f \quad (\text{B.1})$$

whereby the second term in the right hand side of (B.1) represents the additional term as it does not appear in (3.94). Recalling the definition of the damage evolution law (3.24) and the relationship (3.125) between parameter  $\varepsilon_f$  and the characteristic element size  $h$ , (B.1) can be elaborated as:

$$\delta\omega = \frac{\partial g_d}{\partial \kappa_d} \delta\tilde{\varepsilon} + \frac{\kappa_d}{\varepsilon_f^2} \exp\left(-\frac{\kappa_d}{\varepsilon_f}\right) \frac{G_f}{f_i h^2} \delta h \quad (\text{B.2})$$

In order to obtain the perturbation of the characteristic element size, consistent differentiation of (3.122) leads to:

$$\delta h = -h^2 \left( \left[ \sum_{i=1}^{n_c} \frac{\partial N_i(\xi)}{\partial \xi} \delta\tau_i \right] \cdot \frac{\partial \xi}{\partial \mathbf{x}} \cdot \mathbf{n} + \left[ \sum_{i=1}^{n_c} \frac{\partial N_i(\xi)}{\partial \xi} \tau_i \right] \cdot \frac{\partial \xi}{\partial \mathbf{x}} \cdot \delta \mathbf{n} \right) \quad (\text{B.3})$$

From definition (3.123),  $\delta\tau_i$  can be further expanded to:

$$\delta\tau_i = \frac{(\mathbf{x}_i - \mathbf{x}_c) \cdot \delta \mathbf{n} - \tau_{\min} + (\mathbf{x}_i - \mathbf{x}_c) \cdot \mathbf{n} - \delta\tau_{\min}}{\tau_{\max} - \tau_{\min}} - \frac{(\mathbf{x}_i - \mathbf{x}_c) \cdot \mathbf{n} - \tau_{\min}}{(\tau_{\max} - \tau_{\min})^2} (\delta\tau_{\max} - \delta\tau_{\min}) \quad (\text{B.4})$$

whereupon assuming no change of the corner nodes  $(i_{\max}, i_{\min})$  related to the maximum and minimum of  $((\mathbf{x}_i - \mathbf{x}_c) \cdot \mathbf{n})$ , respectively, the following expressions ensue:

$$\begin{aligned}\delta\tau_{\max} &= (\mathbf{x}_{i_{\max}} - \mathbf{x}_c) \cdot \delta\mathbf{n} \\ \delta\tau_{\min} &= (\mathbf{x}_{i_{\min}} - \mathbf{x}_c) \cdot \delta\mathbf{n}\end{aligned}\tag{B.5}$$

As commented in Chapter 3, and originally from Jirásek and Zimmermann (1998a), the perturbation in the first principal direction  $\mathbf{n} = \mathbf{n}_I$  can be expressed as:

$$\delta\mathbf{n}_I = \frac{\delta\gamma_{12}}{2(\varepsilon_{e1}^{tr} - \varepsilon_{e2}^{tr})} \mathbf{n}_{II} + \frac{\delta\gamma_{13}}{2(\varepsilon_{e1}^{tr} - \varepsilon_{e3}^{tr})} \mathbf{n}_{III}\tag{B.6}$$

with  $\delta\gamma_{jk}$  being the engineering shear strains and  $\varepsilon_{ej}^{tr}$  the trial elastic strains, in principal strain base. By resorting to auxiliary vectors:

$$\begin{aligned}\delta_I &= \{0, 0, 0, 1, 0, 0\}^T \\ \delta_{II} &= \{0, 0, 0, 0, 1, 0\}^T\end{aligned}\tag{B.7}$$

and after some elaborations and rearrangements, (B.6) finally transforms into:

$$\delta\mathbf{n}_I = \left[ \frac{\mathbf{n}_{II} \otimes \delta_I}{2(\varepsilon_{e1}^{tr} - \varepsilon_{e2}^{tr})} + \frac{\mathbf{n}_{III} \otimes \delta_{II}}{2(\varepsilon_{e1}^{tr} - \varepsilon_{e3}^{tr})} \right] \cdot \delta\boldsymbol{\varepsilon}\tag{B.8}$$

Lastly, substitution of (B.8) in (B.3) - (B.5) provides a direct relationship between  $\delta h$  and  $\delta\boldsymbol{\varepsilon}$  which, upon its substitution in (B.2), leads to the explicit expression of the perturbation of damage  $\delta\omega$  to be included in the algorithmic elasto-plastic-damage stiffness instead of (3.94).