CONTINUUM APPROACH TO COMPUTATIONAL MULTISCALE MODELING OF PROPAGATING FRACTURE

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Abstract: A new approach to two-scale modeling of propagating fracture, based on computational homogenization (FE2), is presented. The specific features of the approach are: a) a continuum setting for representation of the fracture at both scales based on the Continuum Strong Discontinuity Approach (CSDA), and b) the use, for the considered non-smooth (discontinuous) problem, of the same computational homogenization framework than for classical smooth cases. As a key issue, the approach retrieves an internal/characteristic length computed at the lower scale, which is exported to the upper one and used therein as a regularization parameter for a propagating strong discontinuity kinematics. This guarantees the correct transfer of fracture energy between scales and the proper dissipation at the upper scale. Representative simulations show that the resulting formulation provides mesh objective results with respect to, both, size and bias of the upper-scale mesh, and with respect to the size of the lower-scale RVE/failure cell, as well as the capability to model propagating cracks at the upper scale, in combination with crack-path-field and strain injection techniques. The continuum character of the approach confers to the formulation a minimally invasive character, with respect to standard procedures for computational one-scale homogenization and modeling of propagating material failure.

Keywords: Multi-scale, fracture, propagating failure, continuum strong discontinuity approach

1 Introduction

Multi-scale computational modeling of solids, aiming at improving the predictive capabilities of mechanical models accounting for the description of the material at several scales, is a subject of increasing interest. A number of analytical and computational strategies have been developed in the past considering the description of the constitutive material at different scales, (Hill 1963; Germain 1973; Sanchez-Palencia 1974; Sanchez-Palencia 1980; Michel, Moulinec et al. 1999; Nemat-Nasser 1999; Terada, Hori et al. 2000; Miehe 2002; Dolbow, Khaleel et al. 2004; Miehe and Bayreuther 2007; Vernerey, Liu et al. 2007; Yuan and Fish 2008; Efendiev and Hou 2009; Fish 2009). In most of them, multiscale description of the material itself (e.g. computational material homogenization) and consequences and implications, on the overall modeling of the solid, of this specific
description (computational multiscale modeling), are not generally considered in an integrated setting. In the context of a two scale (macro scale-micro/meso-scale) problem, computational homogenization of materials (FE2) is generally regarded as a way of replacing, at the structural-scale, standard stress-strain phenomenological constitutive models equipped with internal variables, accounting for the micro/mesoscopic material morphology, by point wise overall stress-strain evaluations. The overall stresses are then obtained after solving an auxiliary problem, the homogenization problem, at the micro/meso-scale, in a manifold, the Representative Volume Element (RVE), endowed with a geometrical description of the material morphology. In turn, this RVE problem relies on some well-established paradigms, typically the classical Hill-Mandel principle (Hill 1963; de Souza Neto and Feijoó 2006; de Souza Neto and Feijoo 2008; Geers, Kouznetsova et al. 2010; Blanco, Sánchez et al. 2014) and the strain and stress homogenization concepts. After this, the structural modeling proceeds at the macro/structural scale in a standard manner, with no further modifications.

This weak coupling makes sense for problems involving smooth—linear or nonlinear—material behaviour, but the issue seems not to be so clear for non-smooth responses, like material failure,—typically fracture, de-cohesion, shear banding etc.—where the involved entities (strains, stresses, displacements) can be non-smooth or even unbounded (Oliver and Huespe 2004b). For these non-smooth problems, two options emerge:

a) Use the same homogenization paradigms than for smooth problems, with no specific modification. This approach has been strongly objected: even the existence of the RVE can be questioned, arguing that for fracture cases the material loses the statistical homogeneity (Gitman, Askes et al. 2007), or, from another point of view, that the homogenized constitutive model lacks an internal length (Bazant 2010). A crucial consequence of this issue is the lack of objectivity of the results with respect to the size of the RVE.

b) Modify the homogenization paradigm towards a specific one for non-smooth problems. Selective RVE domain homogenization methods (Kouznetsova, Brekelmans et al. 2001; Kouznetsova, Geers et al. 2004; Belytschko and Song 2010; Nguyen, Lloberas-Valls et al. 2010; Coenen, Kouznetsova et al. 2012) or specific new homogenization paradigms (Sánchez, Blanco et al. 2013; Toro, Sanchez et al. 2014) are possible ways to retrieve RVE-size objectivity of the results. However, sometimes this is done at the cost of a much higher complexity and loss of generality of the approach.

In this context, this work presents a new approach for computational multiscale analysis in non-smooth problems with the following features:

1. Extends the homogenization paradigms for smooth problems—typically the Hill-Mandel principle and the stress-strain homogenization procedures—to non-smooth problems, with no fundamental changes.

2. In both scales, a continuum (stress-strain) constitutive relationship is considered, instead of the most common discrete traction/separation-law, this contributing to provide a unified setting for smooth and non-smooth problems. This is achieved by resorting to the well-established Continuum Strong Discontinuity Approach (CSDA) to material failure (Oliver 1996a; Oliver and Huespe 2004a; Oliver and Huespe 2004b).

3. As for the multiscale modelling issue, it involves a crucial additional entity: an internal (or characteristic) length, which is point wise obtained from the geometrical features of the failure mechanism developed at the low scale. Introduction of an
internal length in material homogenization schemes has been claimed as a ineluctable requirement for physical consistency (Bazant 2010), and some approaches to this subject can be found in recent works (Unger 2013). As a specific feature of the presented approach, for the non-smooth case this internal length is exported, in addition to the homogenized stresses and the tangent constitutive operator, to the macro-scale, and considered the bandwidth of a propagating strain localization band, at that scale.  

4. Consistently with this internal length, a specific computational procedure, based on the crack-path-field and strain injection techniques, recently developed by the authors (Oliver, Dias et al. 2014), is then used for modelling the onset and propagation of this localization band, at the macro-scale. This ensures the macro-scale mesh-size and micro-scale RVE-size objectivity of the results, and the proper energy dissipation at both scales.

In the remaining of this work a detailed description of the mechanical and computational elements of the proposed approach are presented. In section 2, the multi-scale framework and the corresponding homogenization procedure, are described, whereas in section 3 material failure propagation issues are addressed. Section 4 is devoted to present some representative numerical simulations to assess the performance of the proposed approach, and finally, in section 5, some concluding remarks are stated.

Not to distract the reader's attention on issues that, though being crucial for the completeness of the work and the reproducibility of the results, are not in the core of the proposed approach, some appendices are added at the end of the work. Appendix I, details a very simple technique for removing possible spurious unstable modes of the failure cell. Appendix II, refers to the extension to multi-scale problems of the crack-path-field and strain injection techniques, developed by the authors in previous works (Oliver, Dias et al. 2014) for the purposes of modelling the intra-elemental propagation of strong discontinuities in mono-scale problems.

2 Multi-scale modelling setting

2.1 Macroscopic scale

Let us considered the body, $B$, at the macroscopic (structural) scale (see Figure 1). It is assumed that material points, $\mathbf{x}$, of the body belong, at the current time $t$, to either of the two different subdomains (see Figure 1):

![Macroscopic (structural scale) body B: a) subdivision in a non-smooth domain, $B_{loc}(t)$, and a smooth domain $B \setminus B_{loc}(t)$, b) $h$-regularized, displacement and strain, discontinuity kinematics.](image)
• Domain $B \setminus B_{loc}(t)$: the set of points at the macroscale, exhibiting smooth behaviour at the current time. The infinitesimal strain field $\varepsilon(x,t)$ is described, in rate form, as

$$\dot{\varepsilon}(x,t) = (\nabla_x \otimes \dot{u}(x,t))^S \equiv \nabla_S^S \dot{u}(x,t) \quad \forall x \in B \setminus B_{loc}(t)$$

(1)

where $u(x,t)$ is the macroscale displacement field, $t$ stands for the time or pseudo-time parameter and $(\cdot)^S$ stands for the symmetric counterpart of $(\cdot)$.

• Domain $B_{loc}(t)$: the set of points exhibiting material failure and, therefore, some type of unsmooth behaviour at the current time. The strain field at these points is assumed to be captured by a $h$-regularized strong/weak discontinuity kinematics, $h$ being the width of the corresponding strain localization band (see Figure 1-b):

$$\dot{\varepsilon}(x,t) = \tilde{\varepsilon}(x,t) + \frac{\kappa_{B_{loc}}(x)}{h} \gamma(x,t) = \tilde{\varepsilon}(x,t) + \delta_S^h(x) \gamma(x,t) \quad \forall x \in B_{loc}(t)$$

(2)

where $\tilde{\varepsilon}(x,t)$ stands for regular (smooth) counterpart of the strain, $\kappa_{B_{loc}}$ is a colocation (characteristic) function on $B_{loc}$ ($\kappa_{B_{loc}}(x) = 1 \forall x \in B_{loc}$; $\kappa_{B_{loc}}(x) = 0 \forall x \notin B_{loc}$), so that the term $\delta_S^h(x)$ becomes a $h$-regularized Dirac’s delta function shifted at the center-line, $S(t)$ (the macroscopic discontinuity-path at the current time), of band $B_{loc}(t)$ (see Figure 1-(a)). Thus, in equation (2), the term $\delta_S^h(x) \gamma(x_{S,t})$ is the non-smooth (discontinuous and $h$-regularized) localized counterpart of the strains; a space-discontinuous symmetric, second order tensor for the weak-discontinuity case. For the strong-discontinuity case -- stemming from a discontinuous displacement field-- it takes the following specific format of a rank-one tensor, in terms of the macroscopic displacement jump at $S(t)$, $\beta(x_{S,t})$, and the normal to the discontinuity path, $n(x_{S})$:

$$\dot{\varepsilon}_m(x,t) = (\tilde{\varepsilon}_m(x,t) \odot n(x_{S}))^S = \hat{\varepsilon}_m(x,t) (m \otimes n)^S$$

(3)

where notation $(m \otimes n)^S \equiv m \otimes^S n = \frac{1}{2} (m \otimes n + n \otimes m)$ is used to denote the symmetric part of the tensor product $m \otimes n$. Transition, for a given material point, $x$, from the weak discontinuity kinematics, in equation (2), to the strong discontinuity kinematics, in equation (3), is explained in detail in section 2.5.

2.2 Microscopic scale

Let us now assume that the non-smooth behaviour at the structural scale is produced, in turn, by a non-smooth behaviour at the microscale level arising from some type of material failure at this lower scale. Therefore, the next issue is to endow the low-scale model with mechanisms to capture the onset and propagation of this material failure: typically discontinuous micro-displacement fields. For the sake of simplicity, and without prejudice to introduce further, more complex, options, it is considered that the microstructure is able to capture some dominant failure mechanisms of the material. For this purpose, a micro-failure-cell$^1$, $B_m(x)$, of typical size $h_m$, is considered to exist at every material point $x \in B$ (see Figure 2). It accounts for the material morphology at the lower scale (voids, inclusions etc.) as in regular homogenization procedures, but in addition, it is

$^1$ From now on, sub-index $(\cdot)_m$ will denote entities associated to the micro-scale.
endowed with of a set of cohesive bands, $B_{\mu,coh} \subset B_{\mu}$, of very small bandwidth ($k \ll h_{\mu}$), whose position and other geometric properties (typically the normal $n_{\mu}$, see Figure 2) are predefined. Activation (de-cohesion) at the current time, $t$, of a number of those bands, defines the current subset of active bands, $B_{\mu,act}(t) \subset B_{\mu,coh} \subset B_{\mu}$ which constitutes the microscopic failure mechanism at the current time. There is, in principle, no limitation on the number of the bands at the failure cell, though their number and position have to be sufficient to capture the dominant material failure mechanisms at the macro-scale. In consequence, the following domains at the microscale are considered (see Figure 2):

- **Domain $B_{\mu} \setminus B_{\mu,coh}$**: the set of microscopic points, $y$, out of the cohesive bands. They are imposed to exhibit a smooth behaviour described by a continuum elastic model, typically:
  \[
  \sigma_{\mu}(x,y,t) = \Sigma^{elastic}(\varepsilon_{\mu}) \equiv C_{\mu}(y) : \varepsilon_{\mu}(x,y,t) \quad \forall x \in B \setminus B_{\mu,coh} \]
  where $\sigma_{\mu}$ and $\varepsilon_{\mu}$ stand, respectively, for the microscopic stresses and strains at the micro-scale point, $y$, of the failure cell corresponding to the macro-scale point, $x$, and $C_{\mu}(y)$ is the microscopic elastic constitutive tensor.

- **Domain $B_{\mu,coh}$**: the set of microscale cohesive bands. As for the material behaviour, in this case one has to make distinction of two cases:
  a) The failure cell, $B_{\mu}(x)$, corresponds to a non-smooth material point at the macro-scale ($x \in B_{loc}(t)$). Without prejudice of using any other inelastic constitutive model, in the remaining of this work an isotropic continuum damage model, exhibiting $k$-regularized strain softening inelasticity only for tensile stresses—isotropic continuum damage model (Oliver, Huespe et al. 2006)— will be considered. It reads:
  \[
  \sigma_{\mu}(x,y,t) = \Sigma^{inelastic}(\varepsilon_{\mu},r_{\mu}) \equiv (1 - d_{\mu}(r_{\mu}(y,t))) C_{\mu} : \varepsilon_{\mu}(x,y,t) \]
  $x \in B_{loc}(t) \forall y \in B_{\mu,coh}$
  where $d_{\mu} \in [0,1]$ is the, scalar, damage variable whose evolution is described in terms of the internal variable $r_{\mu}$. More details about the model are given in BOX 2-1.
  b) The failure cell, $B_{\mu}(x)$, corresponds to a smooth material point at the macro-scale, ($x \in B \setminus B_{loc}(t)$). In this case, the inelastic model, in equation (5) is enforced to behave instantaneously elastically at the cohesive bands domain, $B_{\mu,coh}$, i.e.:

![Figure 2. Multiscale model: failure-cell with cohesive bands.](image-url)
\( \sigma_i = (1 - d_i) C_i : \varepsilon_i = \frac{q_i}{r_i} C_i : \varepsilon_i \)

\( d_i = \frac{1}{r_i} - \frac{q_i}{r_i} \geq 0 \)

\( r_i = \lambda \)

\( q_i = k \tilde{H}(r_i) \)

\( k \) regularization parameter (bandwidth of localized strains)

\( \tilde{H}(r_i) = \frac{-r_i^2}{2G_i} \) bilinear softening

Intrinsic softening modulus

\( g(e_i, r_i) = \sqrt{\sigma_i^+} = \sigma_i - \sigma_i^+ \)

\( \sigma_i^+ = \{ \sigma_i \} e_i \otimes e_i \)

\( \bar{\sigma}_{i,j} \) principal stress "i"

\( \varepsilon_i \) principal direction "i"

\( \dot{\lambda} \geq 0 \), \( g \leq 0 \), \( \dot{\lambda} g = 0 \)

Karush-Kuhn-Tucker

(loading/unloading) conditions

**Material parameters**: ultimate stress \( \sigma_{\mu}^u \), Young’s modulus \( E_{\mu} \), Poisson ratio \( \nu_{\mu} \), fracture energy \( G_f^\mu \).

\( \sigma_i^+ \) is the positive part of the microscopic effective stress, \( d_i \) is the damage variable and \( r_i \) and \( q_i \) are, respectively, the strain-like and stress-like internal variables.

**REMARK 2.1**: Notice that, according to the previous setting, *the same material morphology is considered at all \( B_\mu(x) \) both for \( x \in B_{loc} \) (failure cell) or \( x \in B \), RVE, the only difference being the considered constitutive behaviour at the cohesive bands, \( B_{\mu,coh} \), defined in equations (5) and (6).

Let us now consider the micro displacement field, \( u_\mu \), at the cell described as

\( u_\mu(x,y,t) = u(x,t) + \varepsilon(x,t) \cdot y + \bar{u}_\mu(y,t) \)

where \( u(x,t) \) and \( \varepsilon(x,t) \) are, respectively, the macroscale displacements and strains at point \( x \) in \( B \), and \( \bar{u}_\mu \) are the microscale displacement fluctuations. Considering a local coordinate system \((\xi, \eta)\) aligned with the domain \( B_{\mu,coh} \) (see Figure 2), the smooth part of the microfluctuation field, \( \bar{u}_\mu \), is defined as:
\[ \tilde{\mathbf{u}}_{k}(\xi, \eta, t) = \mathbf{u}_{k}(\xi, \eta, t) - \mathcal{H}_{B_{k,coh}}(\xi) \beta_{k}(\eta, t) \quad (a) \]

\[ \mathcal{H}_{B_{k,coh}}(\xi) = \begin{cases} 
0 & \forall \mathbf{y} \in (\mathcal{B} \setminus \mathcal{B}_{k,coh})^- \\
\frac{\xi}{k} & \forall \mathbf{y} \in \mathcal{B}_{k,coh} \\
1 & \forall \mathbf{y} \in (\mathcal{B} \setminus \mathcal{B}_{k,coh})^+ 
\end{cases} \quad (b) \]

\[ \beta_{k}(\eta(\mathbf{y}), t) \bigg|_{\mathbf{y} \in \mathcal{B}_{k,coh}} = [\tilde{\mathbf{u}}_{k}(\xi, \eta, t) ]^+ \quad (c) \]

where \( \mathcal{H}_{B_{k,coh}}(\xi) \) is the \( k \)-regularized Heaviside function shifted to \( \mathcal{B}_{k,coh} \), and \( \beta_{k}(\xi, \eta) \) is a (smooth) function arbitrarily defined excepting for the restriction in equation (8)-(c).

Notation \( \big[ (\bullet)(\xi, \eta) \big]^+ \equiv (\bullet)(\xi, \eta) \big|_{k=+} - (\bullet)(\xi, \eta) \big|_{k=-} \) stands for the apparent jump of \( (\bullet)(\xi, \eta) \) between both sides of the cohesive band. From equations (8) it turns out,

\[ [\tilde{\mathbf{u}}_{k}]^+ = [\mathbf{u}_{k}]^+ - [\mathcal{H}_{B_{k,coh}}]^+ [\tilde{\mathbf{u}}_{k}]^+ = 0 \quad (9) \]

and, therefore, function \( \tilde{\mathbf{u}}_{k} \) in equation (8) is smooth. Finally, from equation (8)-(a),

\[ \tilde{\mathbf{u}}_{k}(\mathbf{y}, t) = \mathbf{u}_{k}(\mathbf{y}, t) + \mathcal{H}_{B_{k}}(\mathbf{y}) \beta_{k}(\mathbf{y}, t) \quad (10) \]

(see a sketch in Figure 3). Equation (10) constitutes the displacement counterpart of a \( k \)-regularized strong discontinuity kinematics (Oliver 1996a), and proves that the cohesive bands-approach, herein proposed for the description of material failure at the microstructure, is consistent with consideration of a \( k \)-regularized strong discontinuity at the cohesive domain \( \mathcal{B}_{k,coh} \).

In this context, one can resort to the well-established connection of the continuum modelling of material failure—based on stress-strain constitutive equations equipped with strain softening—and the discrete cohesive fracture mechanics, established in the Continuum Strong Discontinuity Approach (CSDA) to material failure (Oliver, Huespe et al. 2002). This states the equivalence, in the limit \( k \to 0 \), of the proposed approach and the one based on cohesive lines endowed with traction separation laws (Oliver 2000).

![Figure 3. Micro-displacement fluctuation fields.](image)

From equation (10) one obtains,
\[ \nabla^S \tilde{u}_p(y,t) = \nabla^S \tilde{u}_p(y,t) + \mathcal{H}_{\beta} \nabla^S \beta_p(y,t) + (\beta_p \otimes n_p)^S(y_S,t) = \]
\[ = \tilde{\varepsilon}_p(y,t) + \delta^{k}_{S_p}(y,t)(\beta_p \otimes n_p)^S(y_S,t) \quad (a) \]
\[ \varepsilon_p(y,t) = \nabla^S \tilde{u}_p(y,t) + \mathcal{H}_{\beta} \nabla^S \beta_p(y,t) \quad (b) \]
\[ \delta^{k}_{S_p}(y,t) = \frac{1}{k} \kappa_{\beta} \quad (c) \]

where \( \kappa_{\beta}(y) \) is the characteristic (colocation) function in equation (2) so that \( \delta^{k}_{S_p}(y,t) \) becomes a \( k \)-regularized Dirac’s delta function placed at the center line, \( S_p \), of \( B_{\beta, \delta} \). From equations (7) and (11), the micro-strains \( \varepsilon_p \) can be written in terms of the macro-strains, \( \varepsilon(x,t) \), and the micro-fluctuations, \( \tilde{u}_p(y,t) \), as follows:

\[ \varepsilon_p(x,y) = \varepsilon(x) + \nabla^S \tilde{u}_p(y) = \varepsilon(x) + \tilde{\varepsilon}_p(y) + \delta^{k}_{S_p}(\beta_p \otimes n_p)^S(y) \quad (12) \]

Equation (12) displays the classical format of a strain field in a \( k \)-regularized strong discontinuity kinematics, where the second term at the right-hand side becomes unbounded in the limit \( k \to 0 \).

### 2.3 Homogenization procedure

At this point, the RVE/failure-cell homogenization setting is tackled. It has to be emphasized that, in the proposed approach, the homogenization setting is the same for smooth, \( x \in B \setminus B_{\text{loc}}(t) \), and non-smooth, \( x \in B_{\text{loc}}(t) \), material points of the macroscale and it coincides with the one considered in standard smooth settings (de Souza Neto and Feijóo 2006). Therefore, it relies on the following paradigms:

1. **Micro-strain homogenization.**

According to this, the average value, over \( B_p \), of the micro-strains, \( \varepsilon_p(x,y) \), in equation (12) has to be equal to the macro strains, \( \varepsilon(x) \) i.e.

\[ \varepsilon(x) = \frac{1}{\Omega_p} \int_{B_p} \varepsilon_p(x,y) dB \quad (13) \]

where \( \Omega_p = \text{meas}(B_p) \) stands for the area/volume of the failure cell. Replacing equation (12) into (13) results

\[ \varepsilon(x) = \varepsilon(x) + \frac{1}{\Omega_p} \int_{B_p} \nabla^S \tilde{u}_p(y) dB \quad (14) \]

which is satisfied if

\[ \int_{B_p} \nabla^S \tilde{u}_p(y) dB = \int_{\Gamma_p} (\tilde{u}_p(y) \otimes v_p(y))^S d\Gamma = 0 \quad (15) \]

where \( v_p(y) \) stands for the outward normal to the failure cell, and \( \Gamma_p \equiv \partial B_p \) is its boundary (see Figure 2). Thus, we define the space, \( \mathcal{V}_p \), of kinematically admissible micro-displacement fluctuations, as

\[ \text{From now on, dependence on time, } t, \text{ will be omitted excepting when strictly necessary.} \]
Notice that the definition in equation (16) coincides exactly, for this proposed non-smooth setting, with the one considered for standard homogenization in smooth settings (de Souza Neto and Feijóo 2006) and minimum kinematic constraint conditions.


The balance of the macroscopic and microscopic stress power reads
\[ \sigma(x) : \dot{\varepsilon}(x) = \frac{1}{\Omega_m} \int_{B_m(x)} \sigma_{\mu}(x,y) : \dot{\varepsilon}_{\mu}(x,y) dB = \]
\[ = \frac{1}{\Omega_m} \int_{B_m(x)} \sigma_{\mu} : (\dot{\varepsilon}(x) + \nabla s \hat{\mu}(y)) dB \quad \forall \hat{\varepsilon}, \hat{\mu} \in \mathcal{V}_m \]
(17)
which, for arbitrary variations \( \hat{\varepsilon} \neq 0 \); \( \hat{\mu} \neq 0 \) yields
\[ \sigma(x) = \frac{1}{\Omega_m} \int_{B_m(x)} \sigma_{\mu}(x,y) dB \]
(18)
and, for arbitrary variations of \( \hat{\varepsilon} \equiv 0 \); \( \hat{\mu} \neq 0 \), leads to the self-equilibrated stress equation in variational form:
\[ \int_{B_m} \nabla s \hat{\mu} : \sigma_{\mu}(\varepsilon + \nabla s \hat{\mu}) dB = 0 \quad \forall \delta \hat{\mu} \in \mathcal{V}_m \]
(19)
Again, it should be noticed that equations (18) and (19) have the same format than for the smooth case.

2.4 Homogenized constitutive model at the macroscale

Let us consider the failure cell displayed in Figure 4. For the sake of generality, we will consider the cell composed of a matrix and inclusions (or voids), in addition to a number of cohesive bands defining the set \( B_{\mu,coh} \). Among them, there are \( n_{active} \) cohesive bands \( B_{\mu,act}^{(i)} \); \( i = 1...n_{active} \), which are in an inelastic softening state, defining a specific failure mode, \( B_{\mu,act} \subset B_{\mu,coh} \), at the micro-cell. Let us also denote by \( S_{\mu}^{(i)} \) the midline in the cohesive band \( i \) (see Figure 4).

Figure 4. Multiscale model: (a) failure cell with inclusions and cohesive bands; (b) geometrical characterization of the failure mode at the microscale.

\[ \mathcal{V}_m = \{ \hat{\mu} | \int_{\Gamma_m} (\hat{\mu} \otimes \nu_{\mu})^S d\Gamma = 0 \} \]
(16)
Therefore, it is fulfilled
\[ B_{i,act} = \bigcup_{i=1}^{i=n_{active}} B_{i,act}^{(i)} ; \quad S_{i} = \bigcup_{i=1}^{i=n_{active}} S_{i}^{(i)} \]  \hspace{1cm} (20)
where \( S_{i} \) can be regarded as the active failure/crack path at the micro-scale. From equations (10) and (11), one can write
\[ \nabla^{t} \mathbf{u}_{m}(y) = \mathbf{E}_{m}(y) + \delta_{S_{i}}^{(m)}(\beta_{m} \otimes \mathbf{n}_{m})^{S}(y) \]  \hspace{1cm} (a)
\[ \nabla^{t} \mathbf{u}_{m}(y) = \mathbf{E}_{m}(y) + \delta_{S_{i}}^{(m)}(\beta_{m} \otimes \mathbf{n}_{m})^{S}(y) \]  \hspace{1cm} (b)
In this context, the following Lemma can be stated:

**LEMMA:**
\[ \int_{B_{m}} \mathbf{e}_{m}(x,y)dB_{m} = -\int_{S_{i}} (\beta_{m} \otimes \mathbf{n}_{m})^{S}(y)dS \]  \hspace{1cm} (22)

**PROOF:**
Replacement of equation (21) into equation (15) yields,
\[ \int_{B_{m}} \nabla^{t} \mathbf{u}_{m}(y)dB = 0 \Rightarrow \]
\[ \Rightarrow \int_{B_{m}} \mathbf{e}_{m}(y)dB + \int_{B_{m}} \delta_{S_{i}}^{(m)}(\beta_{m} \otimes \mathbf{n}_{m})^{S}(y)dB = \]
\[ = \int_{B_{m}} \mathbf{e}_{m}(y)dB + \int_{S_{i}} (\beta_{m} \otimes \mathbf{n}_{m})^{S}(y)dS = 0 \]  \hspace{1cm} (23)
where condition, in the limit \( (k \to 0) \),
\[ \int_{B_{m,coh}} \delta_{S_{i}}^{(m)}(\bullet)(y)dB \approx \int_{S_{i}} (\bullet)(y)dS \]  \hspace{1cm} (24)
for sufficient regular functions, \( (\bullet)(y) \), has been considered. Equation (23) proofs trivially Lemma (22).

Let us now compute the rate of homogenized stresses in equation (18), in the limit \( k \to 0 \) as
\[ \sigma(x) = \frac{1}{\Omega_{m}} \int_{B_{m}} \mathbf{e}_{m}dB = \frac{1}{\Omega_{m}} \left[ \int_{B_{m}} \mathbf{e}_{m}dB + \int_{B_{m,coh}} \mathbf{e}_{m,coh}dB \right] = \]
\[ = \frac{1}{\Omega_{m}} \int_{B_{m} \setminus B_{m,coh}} \mathbf{C}_{m} : \mathbf{e}_{m,coh}dB \]  \hspace{1cm} (25)
where the bounded character of the micro-stresses, \( \mathbf{\sigma}_{m} \), in \( B_{m,coh} \), and the elastic constitutive model in \( B_{m} \setminus B_{m,k} \) (see equation (4)) have been considered. Now inserting equation (12), for \( y \in B_{m} \setminus B_{m,k} \), into equation (25) yields
\[ \dot{\sigma}(x,t) = \frac{1}{\Omega_{m}} \int_{B_{m} \setminus B_{m,coh}} \mathbf{C}_{m} : (\dot{\mathbf{e}} + \mathbf{\tilde{e}}_{coh})dB \]  \hspace{1cm} (k \to 0) \approx \frac{1}{\Omega_{m}} \int_{B_{m}} \mathbf{C}_{m}(y) : (\dot{\mathbf{e}}(x) + \mathbf{\tilde{e}}_{m}(x,y))dB \]  \hspace{1cm} (26)
where, again, the smooth character of the smooth strains \( \dot{\mathbf{e}} \) and \( \mathbf{\tilde{e}}_{coh} \) has been considered. Equation (26) can be rephrased in terms of the average value of the micro-elastic constitutive tensor \( \mathbf{\overline{C}} \), as:
\[
\mathbf{\sigma}(\mathbf{x}, t) = \frac{1}{\Omega_\mu} \int_{B_\mu} \mathbf{C}_\mu(\mathbf{y}) \mathbf{d}B : \mathbf{\varepsilon}(\mathbf{x}) + \frac{1}{\Omega_\mu} \int_{B_\mu} \mathbf{C}_\mu(\mathbf{y}) : \mathbf{\varepsilon}_i(\mathbf{x}, \mathbf{y}) \mathbf{d}B = \mathbf{\mathcal{C}} \mathbf{\varepsilon} + \frac{1}{\Omega_\mu} \int_{B_\mu} \mathbf{\mathcal{C}} : \mathbf{\varepsilon}_i \mathbf{d}B + \frac{1}{\Omega_\mu} \int_{B_\mu} (\mathbf{\mathcal{C}} - \mathbf{\mathcal{C}}) : \mathbf{\varepsilon}_i \mathbf{d}B 
\]

(a)

\[
\mathbf{\mathcal{C}} \equiv \frac{1}{\Omega_\mu} \int_{B_\mu} \mathbf{C}_\mu(\mathbf{y}) \mathbf{d}B 
\]

(b)

Now, replacing equation (22) into equation (27) yields,

\[
\mathbf{\sigma}(\mathbf{x}, t) = \mathbf{\mathcal{C}} : \mathbf{\varepsilon} - \mathbf{\mathcal{C}} : \mathbf{\varepsilon}_i = \mathbf{L}_p (\mathbf{\mathcal{C}} : \mathbf{\varepsilon}_i) = \mathbf{\mathcal{C}}(x, t) 
\]

(28)

where \( L_p = |S_p| \) is the measure (length in 2D, area in 3D) of \( S_p \) and \( \mathbf{\mathcal{C}}(x, t) \) stands for the average value of \( \mathbf{\varepsilon} \) in the activated macroscopic failure mechanism along the crack path \( S_p \).

Equation (28) can be, then, rephrased giving rise to the homogenized constitutive model in BOX 2-2.

**BOX 2-2: Homogenized constitutive model at the macro-scale**

| homogenized constitutive equation (rate form) | \[ \dot{\mathbf{\sigma}}(\mathbf{x}, t) = \mathbf{\mathcal{C}} : [\dot{\mathbf{\varepsilon}}(\mathbf{x}, t) + \dot{\mathbf{\varepsilon}}(\mathbf{x}, t)] = \mathbf{C}_{hom}^{tang} : \dot{\mathbf{\varepsilon}}(\mathbf{x}, t) \] (a) |
| averaged elastic constitutive tensor | \[ \mathbf{\mathcal{C}} = \frac{1}{\Omega_\mu} \int_{B_\mu} \mathbf{C}_\mu(\mathbf{y}) \mathbf{d}B \] (b) |
| smooth internal strain | \[ \dot{\mathbf{\varepsilon}}(\mathbf{x}, t) = \frac{1}{\Omega_\mu} \int_{B_\mu} \mathbf{C}_\mu^{-1} : \dot{\mathbf{\varepsilon}}(\mathbf{u}) \mathbf{d}B = \mathbf{M}(\mathbf{\varepsilon}(\mathbf{x}, t)) \] (c) |
| non-smooth (localized) internal strain | \[ \dot{\mathbf{\varepsilon}}(\mathbf{x}, t) = \frac{1}{\ell_p} \mathbf{\varepsilon}(\mathbf{x}, t) \] (d) |

In equation (29)-(a), \( \mathbf{C}_{hom}^{tang} \) stands for the macroscale homogenized tangent constitutive operator, which can be point-wise obtained from a standard homogenization procedure, see (Peric, Neto et al. 2011). In equation (29)-(c) \( \mathbf{I} \) is the fourth order symmetric unit tensor and \( \mathbf{A}(\mathbf{y}, \mathbf{\varepsilon}) \) is a strain-concentration like tensor stemming from a standard homogenization of the constitutive behaviour at the domain \( B_\mu \).
Equations in BOX 2-2 display, in an incremental (rate) form at, the macroscopic constitutive model inherited by the macro-scale from the homogenization procedure at the micro-scale. Although that model will not be used for computational purposes\textsuperscript{4}, it supplies relevant insights on the properties of the resulting homogenized constitutive model and crucial requirements on the numerical model for the propagating material failure at the macro-scale, i.e.:

- Equation (29)-(a) corresponds to an inelastic constitutive equation in terms of the average elastic constitutive tensor, $\overline{C}$, at the microscale, see equation (29)-(b), and some inelastic strains, $\dot{\chi}(x,t)$ and $\varepsilon^{(i)}(x,t)$, which would play the role of internal variables in phenomenological models. The evolution equations for those internal variables are given by equations (29)-(c) and (29)-(d). Unlike in phenomenological models, their evolution is determined, at every macroscopic sampling point, $x$, by homogenized values of entities at the corresponding micro-scale failure cell, $B_x(y) : i.e.$

  $\overline{C}_\mu(y,t), \beta_\mu(y,t), \varepsilon(x,t)$, the elastic properties at the micro-scale, $\overline{C}_\mu(y)$ and the specific failure mechanism activated at the micro-scale, $S_x(y)$. This extends to non-smooth problems, some theoretical results already derived for smooth problems, see for instance (Michel and Suquet 2003; Michel and Suquet 2004).

- An internal length $\ell_\mu(x,t)$ emerges naturally in equation (29)-(d). If $n_{dim} \in \{2,3\}$ is the dimension of the problem then, $\ell_\mu$ is the ratio of the measure of the failure cell, $|B_\mu| = \Omega_\mu = O(h_{\mu}^{n_{dim}})$, and the measure (length/surface) of the activated micro-failure mechanism, $L_\mu = |S_\mu| = O(h_{\mu}^{(n_{dim}-1)})$. In consequence $\ell_\mu$ is of the order of the failure-cell size i.e. $\ell_\mu = O(h_{\mu})$. If we assume scale separation, $h_{\mu} \ll L$ (see Figure 1), then $\ell_\mu$ is a very small number in the upper scale $\ell_\mu(x,t) \ll L$ (see Figure 1 and Figure 4).

- Equations (29) can be specified for the domains $B_{loc}(t)$ and $B \setminus B_{loc}(t)$ at the macro scale as:

  1) *Smooth domain $B \setminus B_{loc}(t)$:*  
  The microscale behaviour is instantaneously elastic (see equations (4) and (6)) and, therefore, $\beta_\mu(y,t) = 0 \ \forall y$. Then, in equation (29)-(d), $\varepsilon^{(i)}(x,t) = 0$ and equations (29)-(a) and (29)-(c) read

  $\dot{\varepsilon}(x,t) = \overline{C} : [\dot{\varepsilon}(x,t) + \dot{\chi}(x,t)]$ \hspace{1cm} (a)

  $\dot{\chi}(x,t) = \mathcal{M} : \dot{\varepsilon}(x,t)$ \hspace{1cm} (b)

  and, therefore,

  $\dot{\sigma}(x,t) = \overline{C} : (I + \mathcal{M}) : \dot{\varepsilon}(x,t) = \overline{C}_{\text{hom}}^{\text{elas}} : \dot{\varepsilon}(x,t)$ \hspace{1cm} (30)

- Instead, the homogenized value of the stresses in equation (18) is point-wise used to evaluate the current macro-stresses in terms of the corresponding macro-strains.

\textsuperscript{4} Instead, the homogenized value of the stresses in equation (18) is point-wise used to evaluate the current macro-stresses in terms of the corresponding macro-strains.
where $\overline{C}_{\text{hom}}$ stands for the homogenized elastic constitutive operator at the failure cell $B_{\mu}$.

Notice, from equation (30)-(a), that a bounded strain, $\hat{\varepsilon}(x,t) = \tilde{\varepsilon}(x,t)$ is recovered at $B \setminus B_{\text{loc}}(t)$ as,

$$\hat{\varepsilon}(x,t) = \overline{C}^{-1} : \sigma(x,t) - \dot{x}(x,t) = \tilde{\varepsilon}(x,t) \quad \forall x \in B \setminus B_{\text{loc}}(t)$$

(32)

2) Non-smooth domain $B_{\text{loc}}(t)$:

Material micro-structure displays some failure mechanism by triggering inelasticity (see equations (5)) at the set of activated cohesive bands, $B_{\mu,\text{act}}(x)$. Therefore, $\hat{p}_{\mu}(y,t) = 0 \quad \forall y \in B_{\mu,\text{act}}(x)$ and, from equations (29)-(a) and (29)-(d),

$$\hat{\varepsilon}(x,t) = \overline{C}^{-1} : \sigma(x,t) - \dot{x}(x,t) + \frac{1}{\ell_{\mu}} (\beta_{\mu} \otimes^s n_{\mu})_{S_{\mu}} = \tilde{\varepsilon}(x,t) \quad \text{(bounded)}$$

$$= \hat{\varepsilon}(x,t) + \frac{1}{\ell_{\mu}} (\beta_{\mu} \otimes^s n_{\mu})_{S_{\mu}} \quad \forall x \in B_{\text{loc}}$$

(33)

Equations (32) and (33) can be summarized for the complete domain $B$ as:

$$\hat{\varepsilon}(x,t) = \overline{C}^{-1} : \sigma(x,t) - \dot{x}(x,t) + \frac{K_{\mu}}{\ell_{\mu}} (\beta_{\mu} \otimes^s n_{\mu})_{S_{\mu}} = \tilde{\varepsilon}(x,t)$$

$$\text{(smooth)}$$

$$= \hat{\varepsilon}(x,t) + \frac{K_{\mu}}{\ell_{\mu}} (\beta_{\mu} \otimes^s n_{\mu})_{S_{\mu}} = \hat{\varepsilon}(x,t)$$

(34)

REMARK 2-2. Comparing equation (34) with equation (2), one realizes that the former defines a $\ell_{\mu}$-regularized discontinuity kinematics of bandwidth $h = \ell_{\mu}$. This is a fact of crucial importance for a proper and meaningful modeling of the material failure propagation at the upper scale. In fact, equation (34) suggests that the numerical approach for capturing this propagation has to be consistent with the aforementioned kinematics of regularized strong discontinuity and, more specifically, regularized with the internal length $\ell_{\mu}$.

REMARK 2-3. The role of the internal (or characteristic length), $\ell_{\mu}$, is not only computational, but it has also other relevant physical and mechanical implications. Consideration of such an internal length for multi-scale based approaches has been claimed from the materials mechanics community (Bazant 2010) and introduced in a heuristic way in some previous approaches (Unger 2013).

Remarkably, in the proposed approach, this internal length, $\ell_{\mu}$, is naturally derived from the homogenization setting; it depends on both specific data of the problem and local results of the analysis. For instance: a) the considered macro-scale material point, $x$, b) the microscale length, $h_{\mu}$, c) the morphology at the micro-scale d) the activated failure mechanism at the failure-cell, $S_{\mu}$, which, in turn, depends on d) the history and evolution of the mechanical variables at the micro-scale.
2.5 Time evolution of material failure at the macroscale. Transition from weak to strong discontinuity

Equation (34) corresponds to a specific format of the weak discontinuity kinematics in equation (2) with
\[ \dot{\beta}(x,t) := (\beta_{\mu} \otimes^s \mathbf{n}_{\mu})_{S_{\mu}} = \frac{1}{T_{\mu}} \int_{S_{\mu}} (\beta_{\mu} \otimes \mathbf{n}_{\mu})^S dS \]  
(35)

Since \((\beta_{\mu} \otimes^s \mathbf{n}_{\mu})_{S_{\mu}}\) is not, necessarily a rank-one tensor\(^5\), it does not match necessarily the strong discontinuity kinematics in equation (3) corresponding to a propagating displacement discontinuity, but it evolves towards this situation along time. The time of the analysis, at which equation (35) takes the format
\[ \dot{\beta}(x,t_B) = (\beta_{\mu}(x,t_B) \otimes^s \mathbf{n}_{\mu}(y))_{S_{\mu}} = (\beta(x,t_B) \otimes \mathbf{n}(x))^S = \xi(\mathbf{m} \otimes \mathbf{n})^S = 0 \]  
(36)

will determine the bifurcation time \(t_B(x)\). In other words, the time at which material failure, displaying localized strains in a weak discontinuity format (see equation (2)), starts propagating, as a strong discontinuity, at the considered macro-scale point, \(x\). Determination of this time, and the so-called polarization directions \(n(x)\) and \(m(x)\)\(^6\), is done in the context of the well-known discontinuous bifurcation analysis (Willam and Sobh 1987; Ottosen and Runesson 1991) by solving the problem:

**PROBLEM**

**GIVEN** \(Q_i(x,n) = n \cdot C^{tang}_{\text{hom}}(x,t) \cdot n ; x \in S ; t \in [0,T] \)

**FIND** the first \(t \equiv t_B(x) \in [0,T] \) and all \(n \in \mathbb{I} := \{\mathbf{v} \in \mathbb{R}^{n_{\text{hom}}} | \|\mathbf{v}\| = 1\} \):  
(37)

**FULFILLING** : \(Q_i(x,n) \cdot m = 0 \) for some \(m \in \mathbb{I}\)

where \(C^{tang}_{\text{hom}}\) is the macroscale (homogenized) tangent constitutive (see equation (29)-(a)), \([0,T]\) is the time interval of interest and \(Q_i(x,n)\) is the localization tensor.

A general numerical procedure for solving this problem can be found in (Oliver, Huespe et al. 2010). In general equation (37) provides the bifurcation time, \(t_B(x)\), and two solutions for the normal to the discontinuity path \(S\) (see Figure 1) i.e.: \(n_1(x) \equiv n\), \(n_2(x) \equiv m\).

Now, examining equation (36), one realizes that the equality is fulfilled under the following circumstances:

1) The fluctuations jump at the microscale, \(\dot{\beta}_m\), is spatially constant at the failure-cell:
\[ \dot{\beta}_m(x,y,t) = \dot{\beta}_m(x,t) \forall y \in B_{\mu} \]
\[ \Rightarrow \left\{ (\beta_{\mu} \otimes^s \mathbf{n}_{\mu})_{S_{\mu}} = (\beta_{\mu}(x,t) \otimes \mathbf{n}_{\mu}(x,y))_{S_{\mu}} \right\}^S = \zeta(\beta_{\mu}(x,t) \otimes \mathbf{a}(x))^S \]
(38)

\[ \mathbf{a}(x) = \frac{1}{\zeta} \mathbf{n}_{\mu}(x,y)_{S_{\mu}} ; \|\mathbf{a}\| = 1 ; \zeta(\mathbf{x}) = \left\| \mathbf{n}_{\mu}(x,y)_{S_{\mu}} \right\| = \zeta(\mathbf{n}_{\mu}) \]

where factor \(\zeta(\mathbf{x})\) is a measure of the tortuosity of the activated micro-scale failure path \(S_{\mu}\) (for instance, for \(S_{\mu}\) being a straight line then \(\zeta = 1\)).

Replacing equation (38) into equation (36) yields:

---

\(^5\) Since the sum (integral) of rank-one tensors is not a rank-one tensor.

\(^6\) For symmetric \(C^{tang}_{\text{hom}}\) the problem is indifferent to the order of the couple \((\mathbf{n}, \mathbf{m})\).
\[ \zeta(\hat{\beta}_\mu(x,t) \otimes a(x))^S = (\hat{\beta}(x,t) \otimes n(x))^S \Rightarrow \begin{cases} \hat{\beta}(x,t) = \zeta(n_\mu)\hat{\beta}_\mu(x,t) = \mathcal{F}(n_\mu, \hat{\beta}_\mu) \\ n(x) = a(x) = \frac{1}{\zeta(n_\mu)}(n_\mu)^S = \mathcal{G}(n_\mu) \end{cases} \tag{39} \]

2) The activated failure path at the micro-scale, \( S_\mu \), is a straight line (or a plain surface), with spatially constant normal \( n_\mu \):
\[
n_\mu(x,y) = n_\mu(x) \\
\Rightarrow n(x) = n_\mu(x) ; \quad \hat{\beta}(x,t) = \overline{\hat{\beta}}_\mu(x,y,t) \tag{40} \]

This is an academic case, since it corresponds to a non-realistic morphology of the failure-cell (\( \mathcal{B}_{\mu,coh} \) defines a straight/plane band). Therefore, it will be discarded because of its lack of physical significance and practical interest.

REMARK 2-4. The previous analysis leads to the following statements:

1. The (rate of the) micro-scale displacement-jump function (after bifurcation) is constant across the failure-cell (\( \hat{\beta}_\mu(x,y,t) = \hat{\beta}_\mu(x,t) \)) in equation (38).

2. The (rate of the) macro-scale displacement-jump function, \( \hat{\beta}(x,t) \), (after bifurcation) equals the micro-fluctuation jump, \( \hat{\beta}_\mu(x,t) \), corrected by the (scalar) tortuosity factor (\( \hat{\beta}(x,t) = \zeta(x)\hat{\beta}_\mu(x,t) \) in equation (39)-(a)).

3. After bifurcation, the macroscale normal to the crack-path \( n(x) \) equals the (normalized) average of the normal to the corresponding microscopic failure mechanism \( a(x) = \frac{1}{\zeta(n_\mu)} \overline{n_\mu(x,y)}^S \) in equation (39)-(b)).

4. It should be also noticed another subtle aspect of statements 2 and 3 above. In fact, inspection of equations (36) and (38) reveals that the symmetric operator \( (n \otimes m)^S \) makes the results insensitive with respect to an interchange of vectors \( n \rightleftharpoons m \). Therefore, besides the solutions in equation (39), solutions
\[
\hat{\beta}^*(x) = \|\hat{\beta}_\mu(x)\|a(x) = \|\hat{\beta}_\mu(x)\|\frac{(n_\mu)^S}{\zeta(n_\mu)} = \mathcal{F}^*(\hat{\beta}_\mu, n_\mu) \\
n^*(x) = \frac{1}{\|\hat{\beta}_\mu(x)\|} \hat{\beta}_\mu(x) = \mathcal{G}^*(\hat{\beta}_\mu) \tag{41} \\
\]

fulfilling
\[
(\hat{\beta}^* \otimes n^*)^S = (\hat{\beta}_\mu(x) \otimes (n_\mu)^S)^S = (\hat{\beta} \otimes n)^S = \overline{\beta} \rightleftharpoons \overline{n} \tag{42} \\
\]

are also admissible. In other words, what is relevant for the resulting macroscopic homogenized constitutive model is not the couple \( (n, \hat{\beta}) \) but its symmetric tensor product.
This indifference, with respect to vector swap in \((n \otimes m)^5\), motivates that a given microscopic failure mechanism \(\{n_\mu, \beta_\mu\}\) gives rise to two possible combinations of the macro-scale displacement jump and normal:

\[
\{\beta, n\} \equiv \{\mathcal{F}(n_\mu, \beta_\mu), \mathcal{G}(n_\mu)\}
\]

\[
\{\beta^*, n^*\} \equiv \{\mathcal{F}^*(\beta_\mu, n_\mu), \mathcal{G}^*(\beta_\mu)\}
\]

as in equations (39) and (41). This enriches the modelling capabilities of the approach for propagation directions in the macroscale. Indeed, even with a relatively poor description of the failure mechanisms at the microscopic scale (restricted set of \(n_\mu\)'s but unrestricted set of \(\beta_\mu\)'s) a much wider set of propagation directions \((\{n \mid n = \mathcal{G}(n_\mu)\} \cup \{n^* \mid n^* = \mathcal{G}^*(\beta_\mu)\})\) can be captured at the macro-scale.

These are \textit{a priori} results, not explicitly imposed in the approach, which shall be corroborated by the numerical simulations in section 4.

2.6 Energy dissipation. Fracture energy issues.

The material failure at the micro-cell \(B_\mu\), translates into propagating failure at the macro-scale, which, in turn, is captured through the regularized strain localization band, \(B_{loc}(t)\) (see Figure 4). The proposed approach enforces this bandwidth to be precisely the internal length, \(\ell_{\mu}(x)\) in equation (29)-(d).

Let us consider the fracture energy, \(G^f(y)\), corresponding to points \(y \in B_{\mu,act}\) at the microscale, understood as a material property that can be different for every material compound at the microstructure, and the macro-scale fracture energy, \(G^f(x)\), obtained as an output from the homogenization procedure. According to their definition (expended power per unity of mid-surface of the localization band) those fracture energies can be, respectively computed, in terms of the fracture energy densities\(^7\) (per unit of volume) \(g^f(x)\) and \(g^f_\mu(y)\):

\[
g^f(x) = \frac{G^f(x)}{\ell_{\mu}(x)} = \int_0^\infty \sigma(x, t) : \dot{e}(x, t) dt \quad \forall x \in B_{loc} \quad (a)
\]

\[
g^f_\mu(y) = \frac{G^f_\mu(y)}{k} = \int_0^\infty \sigma_\mu(y, t) : \dot{e}_\mu(y, t) dt \quad \forall y \in B_{\mu,coh} \quad (b)
\]

In this setting, the following Lemma holds:

**LEMMA:** The macroscopic fracture energy, \(G^f(x)\), is the average of the microscopic fracture energy \(G^f_\mu(y)\), along the activated failure mechanism path at the micro-scale, \(S_\mu(x)\) (see Figure 4):

\[
G^f(x) = \int_{S_\mu(x)} G^f_\mu(y) dy
\]

\(^7\) Strictly speaking, the integration of the macroscopic specific fracture energy, \(g^f(x)\) in equation (43)-(a) should be evaluated along the interval \([t_B, \infty]\), where \(t_B(x)\) stands for the macroscopic bifurcation time in equation (37). Nevertheless, here the pre-bifurcation dissipated energy at the macro-scale is considered negligible, so that it is integrated along the interval \([0, \infty]\).
\[ G^f(x) = \frac{1}{\ell_\mu(x)} \int_{S_\mu(x)} G^f_\mu(y) dS_\mu = \frac{G^f_\mu(y)}{\ell_\mu(x)} \quad (45) \]

**PROOF:**
Considering the Hill-Mandel principle in equation (17), equation (44)-(a) reads,
\[ G^f(x) = \int_0^\infty \sigma(x,t) : \dot{\varepsilon}(x,t) dt = \int_0^\infty \frac{1}{\Omega_\mu} \int_{B_\mu} \sigma_\mu(x,y,t) : \dot{\varepsilon}_\mu(x,y,t) dS_\mu dt = \]
\[ = \int_0^\infty \frac{k}{\Omega_\mu} \int_{B_\mu,act} \sigma(x,y,t) : \dot{\varepsilon}_\mu(x,y,t) dS_\mu dt = \]
\[ = \int_{S_\mu} \left[ \frac{k}{\Omega_\mu} \int_{B_\mu,act} \sigma(x,y,t) : \dot{\varepsilon}_\mu(x,y,t) dS_\mu \right] dt = \]
where the fact that, in the domain outside the active bands \( B_\mu \setminus B_{\mu,act} \), the material is elastic (with no dissipation), has been taken into account. Now, inserting equation (44)-(b) into equation (46), and considering the definition of the internal length, \( \ell_\mu \) in equation (29)-(d), yields
\[ \frac{G^f(x)}{\ell_\mu(x)} = \frac{1}{\Omega_\mu} \int_{S_\mu} \left[ \frac{k}{\Omega_\mu} \int_{0}^{\infty} \sigma_\mu(x,y,t) : \dot{\varepsilon}_\mu(x,y,t) dt \right] dS_\mu = \frac{1}{\Omega_\mu} \int_{S_\mu} G^f_\mu(y) dS_\mu = \]
\[ \frac{G^f_\mu(y)}{\ell_\mu(x)} \]
\[ = \frac{L_\mu}{\Omega_\mu} \int_{S_\mu} G^f_\mu(y) dS_\mu = \frac{1}{\ell_\mu(x)} G^f_\mu(y) \quad (47) \]
which proves the Lemma.

**REMARK 2-5.** For homogeneous fracture energy at the active cohesive bands \( G^f_\mu(y) = G^f_\mu \forall y \in B_{\mu,act} \) the lemma, consistently, translates into conservation of the fracture energy along the scales i.e.:
\[ G^f(x) = G^f_\mu \quad (48) \]

The previous results rely crucially on the ability to induce a localization band of bandwidth \( \ell_\mu(x) \) at the macro-scale. This issue is tackled in Appendix II.

### 3 Propagation of material failure

#### 3.1 Propagation of material failure at the micro-scale. Failure cell finite element model.

A standard finite element model is adopted for the numerical simulation of the RVE/failure-cell response. One, quadrilateral\(^8\), finite element is used across the thickness of the cohesive bands \( B_{\mu,coh} \), as shown in Figure 5. The interpolation order along the coordinate \( \eta \) may be arbitrary. However, it must be linear along the coordinate \( \xi \) in order to capture the function \( \mathcal{H}_{\ell_\delta,\lambda}(\eta) \) defined in equation (8)-(b).

---

\(^8\) However, there is no intrinsic restriction for using other options, like triangular elements.
Figure 5. Multiscale model: finite element discretization at the micro-scale.

Propagation of material failure along the cohesive bands takes place, in a natural fashion, as inelasticity is triggered in one element, $B_{\mu,\text{coh}}^{(e)}$, and it propagates across other elements of $B_{\mu,\text{coh}}^{(e)}$. The set of all elements, $e$, of the cohesive bands experiencing inelastic loading at the center point $y_C^{(e)}$ of the element, see Figure 5, determines, at every time, $t$, the failure mechanism at the micro-scale, i.e.:

$$B_{\mu,\text{act}}(t) := \{ \bigcup_{B_{\mu,\text{coh}}^{(e)} \subseteq B_{\mu,\text{act}(x,y)}} \{ y_C^{(e)}, t > 0 \}$$

where the instantaneous inelasticity status (de-cohesion) is evaluated in terms of a positive evolution of the internal variable $\hat{\tau}_m > 0$ (see BOX 2-1).

From equation (49), one can determine the measure (length/surface) of the activated failure mechanism in equation (29)-(d) and the corresponding internal length as

$$L_{\mu}(x,t) = \sum_{\forall B_{\mu,\text{coh}}^{(e)} \subseteq B_{\mu,\text{act}(x,y)}} L_{\mu}^{(e)} \quad (a)$$

$$\ell_{\mu}(x,t) = \frac{\Omega_{\mu}}{L_{\mu}(x,t)} < h^{(e)}(x) \quad (b)$$

where $L_{\mu}^{(e)}$ stands for the individual length of the active element, $B_{\mu,\text{act}}^{(e)}$, in the set of active cohesive bands $B_{\mu,\text{act}}(t)$. In equation (50)-(b), the limitation, $\ell_{\mu}(x,t) < h^{(e)}(x)$ resolves the indetermination for the case that no damage occurs at the micro-scale (i.e. $L_{\mu} = 0$; $\hat{r}(x,y,t) = 0 \ \forall y \in B_{\mu}^{(e)}$).

REMARK 3-1. In practice, dependence on pseudo-time, $t$, of entities $B_{\mu,\text{act}}(t)$, $L_{\mu}(x,t)$ and $\ell_{\mu}(x,t)$ in equation (50) only holds for the time interval $[t_f(x), t_B(x)]$, where $t_f(x)$ stands for the time where material inelasticity onsets at the failure cell, and $t_B(x)$ is the macroscopic bifurcation time in equation (37). At time $t_B(x)$, the failure mechanism at the cell is assumed fully consolidated and $\ell_{\mu}(x,t)$ in equation (50)-(b) is made constant in time and redefined as:

$$\ell_{\mu}(x,t) := \ell_{\mu}(x) = \ell_{\mu}(x,t_B(x)) \ \forall t \geq t_B(x)$$

$h^{(e)}$ is, typically, the directional bandwidth of the corresponding macroscale finite element (see Table 3 in Appendix II.)
3.1.1 Unstable failure modes. Imposition of constant fluctuation jumps at cohesive bands.

Inspection of equations in BOX 2-2 reveals that the model might exhibit some instability. Indeed, the structure of the inelastic strain in equation (29)-(c), allows situations displaying:

\[ \beta_{\mu}(y) = 0 \quad \text{for some } y \in \mathcal{S}_\mu \quad (a) \]

\[ \dot{\varepsilon}^{(i)}(x,t) = \frac{1}{\mu_s} (\beta_{\mu}(x,y) \otimes n_{\mu}(x,y))_{\mathcal{S}_i} = 0 \quad (b) \]

which can give rise to some instabilities in the microscopic failure mechanisms. In Appendix I this issue is studied and a remedy to preclude this instabilities, based on imposing an internal restriction in the fluctuations on some of the cohesive bands, is presented.

3.2 Propagation of material-failure at the macroscale. Crack-path-field and strain injection techniques in multi-scale problems.

A difficult issue in computational modeling of material failure is the appropriate capture of its onset and propagation. Material failure propagation algorithms aim at answering the following two questions: 1) when does failure trigger at a given material point?, and, 2) how does it propagates?

As commented in section 3.1, at the lower scale (failure-cell) where the morphology and position of candidate propagation mechanisms (set \( \mathcal{B}_{\mu,coh} \)) are predefined, this is a minor issue; both questions are automatically answered in terms of when and what cohesive-band elements enter into the softening regime according to equation (49). However, at the upper scale, there is no predefinition of the failure path and, in principle, any material point may fail and propagate in any direction.

To answer the above questions, in this work we have extended, to the multiscale case, a procedure for modeling onset and propagation of discontinuities recently developed by the authors for one-scale problems (Oliver, Dias et al. 2014). The proposed methodology is based on the use of two specific techniques:

1) **Crack-path-field techniques**, consisting of the identification of the trace, during time and across the domain \( \mathcal{B} \), of an evolving strong discontinuity represented by a strain localized field, in the subset \( \mathcal{B}_{id} \subset \mathcal{B} \). The so-called crack path field, \( \mu(x,t) \), is obtained from a selected localized scalar variable, \( \alpha(x,t) \), and its zero level set identifies, at every time \( t \) of the analysis, the domain, \( \Gamma_r \), that contains the crack-path, \( \mathcal{S}_i \). It is computed as:

\[ \mathcal{S}_i \subset \Gamma_r := \left\{ x \in \mathcal{B}_{loc} \mid \mu(x,t) = \frac{\partial \alpha}{\partial \varepsilon} = \nabla \alpha \cdot \dot{\varepsilon}(x,t) = 0 \right\} \quad (53) \]

which identifies the crack path as the locus of the \( e \)-directional maximum of the field \( \alpha(x,t) \) (see Figure 6). The optimum value for the directional unit vector, \( \hat{e}(x,t) \), in equation (53) should be the one orthogonal to the crack path, \( \Gamma_r \), which, in turn is the unknown of the problem. From the authors’ experience, a convenient, approximate, value for \( \hat{e}(x,t) \), is extracted from the gradient of a displacement field scalar measure\(^{10} \), \( a(x,t) \), i.e.:

---

\(^{10}\) This approximately identifies \( e(x,t) \) as the direction orthogonal the localization propagation
\[ e(x,t) = \nabla a(x,t) \]
\[ a(x,t) = \sum_{j=1}^{n_{\text{int}}} \nabla u_j(x,t) \quad ; \quad u_j(x,t) = u(x,t) \cdot \hat{e}_j \]
\[ \dot{e}(x,t) = \frac{e(x,t)}{\|e(x,t)\|} \]

For the present multiscale approach, the localized variable \( a(x,t) \) in equation (53) has to be specifically imported from the microstructure. Here, it is proposed the following definition in terms of the damage variable at the microscale, \( \mu \), in BOX 2-1, i.e. :

\[
\begin{align*}
\dot{\alpha}(x,t) &= \ell_\mu(x,t) \frac{1}{\Omega_\mu} \int_{\Omega_\mu} \dot{\epsilon}_\mu(x,y,t) d\Omega = \frac{1}{L_\mu(x,t)} \int_{\Omega_\mu} \dot{\epsilon}_\mu(x,y,t) d\Omega \quad (a) \\
\alpha(x,0) &= 0 \quad (b)
\end{align*}
\]

where \( \ell_\mu \) is the internal/characteristic length, defined in equation (50)-(b) .

The corresponding algorithm, based on smoothing the variables \( \alpha(x,t) \) and \( \frac{\partial \alpha}{\partial e} \) in equations (53) and (55), is presented in BOX 3-1.

Figure 6. Crack-path-field technique. (a) and (b) evolving crack-path, \( S_t \); (c) and (d) 1D sketch of the algorithm to obtain the crack path field from the smooth derivative of the localized variable \( \alpha \) (see also BOX 3-1).
PROBLEM

GIVEN:
\[ \alpha(x,t) : \mathcal{B} \times [0,T] \to \mathbb{R}^+ \]
\[ \hat{\varepsilon}(x,t) : \mathcal{B} \times [0,T] \to \mathbb{R}^{n_{dim}} = \{ \mathbf{v} \in \mathbb{R}^{n_{dim}} | \| \mathbf{v} \| = 1 \} \]

\[ \mathcal{V} := \{ \eta(x) = \sum_{i=1}^{n_{node}} N_i(x) \eta_i ; \eta \in H^1(\mathcal{B}) \} \]

\[ \lambda_0 := \{ \eta(x) = \sum_{i=1}^{n_{node}} N_i(x) \eta_i ; \eta \in H^1(\mathcal{B}); \eta|_{\partial\mathcal{B}} = 0 \} \]

FIND:
(a) \[ \psi_\tau(x) \in \mathcal{V}_0 \text{ fulfilling } \int_{\mathcal{B}} \psi_\tau (\psi_\tau - \alpha(x,t))d\mathcal{B} = 0 \quad \forall \psi_\tau \in \mathcal{V}_0 \]
(b) \[ \mu_\tau(x) \in \mathcal{V}_0^h \text{ fulfilling } \int_{\mathcal{B}} \mu_\tau (\mu_\tau - \frac{\partial \psi_\tau}{\partial \mathbf{n}})d\mathcal{B} = 0 \quad \forall \mu_\tau \in \mathcal{V}_0^h \]
(c) \[ \Gamma_\tau := \{ x \in \mathcal{B} ; \mu_\tau(x) = 0 \} \rightarrow \text{zero level set of } \mu_\tau(x) \]

2. Strain injection techniques: consisting of the insertion in specific, time-dependent, sub-domains \( B_{\text{inj}}^{(i)}(t) \subset \mathcal{B} \), \( B_{\text{inj}}(t) = \bigcup_{i=1}^{n_{inj}} B_{\text{inj}}^{(i)}(t) \) (see Figure 7), of goal-oriented strain fields. By using strain injection techniques a number of different strain rate patterns, \( \hat{\varepsilon}(x,t) \equiv \hat{\varepsilon}_i(x) \), can be inserted at the specific domains, \( B_{\text{inj}}^{(i)}(t) \), using classical two-field, \( \hat{\varepsilon}_i(x) / \nabla \hat{\varepsilon}_i(x) \) mixed finite element strategies (Zienkiewicz and Taylor 1994). The format of the considered problem in terms of rates (see BOX 3-2), allows keeping the resulting time-varying problem smooth in time, in spite of the, possible, sudden changes of the injected rate-of-strain formats. More details on the technique can be found in a recent work of the authors (Oliver, Dias et al. 2014).

Figure 7. Strain injection: the injection domains, \( B_{\text{inj}}^{(i)}(t) \), are injected an assumed (rate of) strain, \( \hat{\varepsilon}_{\text{inj}}^{(i)}(x,t) \), in the specific time interval \( [\mathcal{I}_{\text{inj}}^{(i)} \subset [0,T] \)
For the purposes of this work, two different injections are carried out: a) weak discontinuity injection and b) strong discontinuity injection. Their essential features for the present multiscale approach are described in detail in Appendix II.

REMARK 3-2. In the context of the strain-injection technique, the localization domain, denoted as $B_{loc}$ in the proposed multi-scale approach (see section 2.1 and Figure 1), becomes the strain-injection domain, $B_{inj} = B_{loc}$ (see Figure 7).

4 Representative simulations

4.1 Objectivity analysis of the proposed multiscale model

Objectivity is here understood as the insensitivity of the numerical solutions with respect to: a) changes in size and bias of the macroscale finite element mesh and, b) changes of the size and shape of the failure-cell adopted for representing the material micro/meso structure.

4.1.1 Objectivity with respect to the macroscale mesh size and bias

Let us consider the 2D strip under uniaxial tensile stretching (in plane strain) depicted in Figure 8, loaded by imposing a horizontal homogenous displacement, $\delta$, at the right edge, while the left edge stays fixed. The strip thickness is 1.0 m.
The three meshes depicted in Figure 9 are considered. For computational saving reasons, the meshes are only modified at the central zone of the strip, i.e. the region where the crack propagates. Meshes (a), (b) and (c) have quadrilateral elements with sizes: \( h^c \approx 0.065m \), \( 0.035m \) and \( 0.024m \) respectively. In addition, multiscale modelling is restricted to the central zone, so that the remaining of the specimen is modeled with the one-scale (elastic) homogenized material.

The mesostructure is assumed composed of a matrix, in plane strain state, with voids of circular shape with arbitrary diameter and space distributions. In Figure 9-(a), the adopted failure cell is displayed. The considered material properties are given in Table 1.

Table 1. Strip under tensile stretch. Material properties.

<table>
<thead>
<tr>
<th></th>
<th>Young Modulus [GPa]</th>
<th>Poisson Ratio</th>
<th>Yield stress [Mpa]</th>
<th>Fracture Energy [Nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>30.</td>
<td>0.15</td>
<td>Elastic</td>
<td>-</td>
</tr>
<tr>
<td>Cohesive bands</td>
<td>30.</td>
<td>0.15</td>
<td>3.</td>
<td>1000.</td>
</tr>
</tbody>
</table>

In order to trigger the crack initiation in the central zone of the strip, one element in every mesh is perturbed (in red in Figure 9), by decreasing in a 25% the ultimate stress at the corresponding microscale cohesive bands.

Figure 9. Objectivity with respect to changes of the finite element mesh at the macroscale. (a) Multiscale model and failure-cell; (b) coarse discretization (58FE, \( h^c \approx 0.065m \)); (c) medium discretization (192FE, \( h^c \approx 0.035m \)); (c) fine discretization (504 FE, \( h^c \approx 0.024m \)).
In Figure 10 the obtained numerical results are displayed. Figure 10-(a) plots the total load $F$ vs. the horizontal displacement $\delta$ for the three meshes. Figure 10-b displays the resulting crack path at the end of the analysis for every mesh.

![Graph showing load vs. displacement](image)

**Figure 10.** Objectivity with respect to changes of the finite element mesh at the macro-scale: (a) reaction force vs. end-displacement; (b) crack path (for meshes a, b and c) and deformed mesoscopic cell displaying the macroscopic failure mechanisms (activated cohesive bands).

The insensitivity of the structural responses in Figure 10-(a), with respect to meshes of different size and bias, proves the mesh objectivity of the model.

### 4.1.2 Objectivity with respect to shape and size of the failure-cell

A basic issue in multiscale material modeling is that the response, displayed by cells representing the microscopic morphology of the material, should be independent of changes in shape and size of these cells, provided they are large enough to characterize the material statistically.

In order to check this specific issue using the proposed approach, the test sketched in Figure 11 is done. A set of different cells is adopted for characterizing the material response. They are constructed from the repetition, in the horizontal and vertical directions, of a basic cell (see Figure 11-(b)).

The macroscale structural problem and the material properties are the same than in section 4.1.1: a strip undergoing tensile loading with multiscale modelling restricted to the central zone (see Figure 11-(a)).

The mesostructure consists of a matrix with a periodic array of cylindrical voids, arranged in a squared pattern of size $h = 0.001m$, see Figure 11-(a). In order to represent this mesostructure, the unit mesoscopic cell, depicted in Figure 11-(b) and denoted (1x1), is used first. Then, two alternative cells, obtained by repeating cell (1x1) in the horizontal and vertical directions, denoted as (2x1) and (2x2) respectively in Figure 11-(a), are additionally used for the multiscale analysis. Under the chosen loading conditions and microstructure failure cell, the microscale failure mode consists, in the three cases, of the activation of a single vertical column of cohesive bands (see Figure 11-(b)), which translates in a macroscale vertical crack at the central part of the strip (see Figure 11-(a)).
Figure 11. Objectivity with respect to changes in the failure-cell. (a) Test description; (b) microcell (1x1); c) Structural responses (load vs. horizontal displacement curves) for mesoscopic failure cells: 1x1, 2x1 and 2x2.

Figure 11-(c) displays the structural response obtained with the three considered mesoscopic cells, (1x1), (2x1) and (2x2), in terms of the load vs. horizontal displacement response. The almost indistinguishable results for the three cases assess the objectivity of the response. In the achievement of these results, it is again emphasized the key role played by the regularization of the kinematics in equation (34), in terms of the microscopic characteristic length $\ell_\mu$ (in equation (50)-(b)). Indeed, this length takes different values in each case, i.e.: $\ell_\mu = h$ for microcell (1x1), and $\ell_\mu = 2h$ for microcells (2x1) and (2x2).

4.1.3 Fracture energy

Next, the value of the macroscale fracture energy, $G^f(\mathbf{x})$, obtained from the analyzes, is compared with the theoretical (analytical) one in equation (45). In order to induce a straight macroscale crack-path with an exactly measurable length, the strip is solved with a vertical structured mesh. As shown in Figure 11-(a), only one row of elements at the central zone of the strip is endowed with a multiscale model. Micro-cell (1x1) is taken and a vertical macroscopic crack develops. The material parameters are the same than in the previous case.

Taking into account that the inner void in the failure cell can be considered as a cohesive band with a null fracture energy and length $meas(A_{coh}^{\text{void}}) = 3/10h$, the average value of the cohesive fracture energy along the developed microscopic failure mechanism is evaluated (see equation (45) and Figure 11-(b)) as:

$$A_{coh}^{\text{eff}} = 0.351 \text{[kN m]}$$
\[ G_{\text{analytical}}^f \equiv G_0^f(y)_{S_p} = \frac{7/10h}{h}G_0^f = 700 \text{N/m} \] (60)

this supplying the analytical value of the overall (macroscopic) fracture energy, \( G_{\text{analytical}}^f \).

In addition, the numerically obtained value of the overall fracture energy, \( G_{\text{numerical}}^f \), can be extracted from the area, \( A_{\text{eff}} \), under the structural force-displacement curve in Figure 11-(c) i.e.:

\[ G_{\text{numerical}}^f = \frac{A_{\text{eff}}}{\text{length}(S) \times \text{thickness}} = \frac{351 \text{Nm}}{0.5 \text{m} \times 1 \text{m}} = 702 \text{N/m} \] (61)

which matches the theoretical value in equation (60).

4.2 Multiscale model assessment: Nooru-Mohamed test

The experimental test on concrete specimens reported by (Nooru-Mohamed 1992), and sketched in Figure 12, is now used to assess the ability of the proposed approach to model propagating material failure at two scales. The adopted failure cell is presented in Figure 12-(b). For computational cost reasons, the cell crudely represents the morphology of concrete as a matrix (mortar) with some inclusions (aggregates) of different sizes. Therefore, no attempt has been done to represent the statistically distribution of heterogeneities and failure characteristics, at the mesoscopic level, observed in standard concretes. The interest is restricted to assess the ability of the numerical model to simulate a rather complex structural behaviour, involving propagating material failure in two scales, and to compare the results with the wide set of experiences available for this benchmark using single scale phenomenological approaches.

4.2.1 Geometrical features and loading paths

The specimen, of size 200 mm \( \times \) 200 mm and 50 mm of thickness, with two notches (25 mm depth and 0.125 depth/with ratio) is depicted in light grey in Figure 12-(a). The dark grey part of the structure is made of steel. It is considered infinitely rigid and used to apply the different loads in a distributed form.

![Figure 12. Nooru-Mohamed test](image)

Loading consists of a shear force applied in a nearly elastic regime, until reaching the value \( P_s = 5\text{kN} \) and remaining constant afterwards. Subsequently, an increasing vertical...
uniformly distributed load $P$ is superposed (see Figure 11-(a)-(c)). During the first loading stage (shear force application), the left and top steel parts are constrained to remain vertical and horizontal, respectively.

4.2.2 Material properties description

The mesoscopic failure cell, depicted in Figure 12-(b), crudely represents a concrete-like material at the mesoscale (matrix/aggregates). Light grey regions represent cohesive/failure bands, medium grey zone stands for the cement-like matrix and dark grey regions represents aggregates (the cohesive bands into the aggregates are inhibited to failure). Material properties of the cell are summarized in Table 2.

<table>
<thead>
<tr>
<th></th>
<th>Young Modulus [GPa]</th>
<th>Poisson Ratio</th>
<th>Ultimate stress [Mpa]</th>
<th>Fracture Energy [N/m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>21.</td>
<td>0.15</td>
<td>Elastic</td>
<td>-</td>
</tr>
<tr>
<td>Cohesive bands</td>
<td>21.</td>
<td>0.15</td>
<td>3.</td>
<td>20.</td>
</tr>
<tr>
<td>Aggregates</td>
<td>100.</td>
<td>0.15</td>
<td>Elastic</td>
<td>-</td>
</tr>
</tbody>
</table>

4.2.3 Crack propagation result

In order to analyze the ability of the proposed approach for capturing the crack evolution, attention is first focused on the macroscopic scale. In Figure 13, the iso-displacement contours at the end of the simulation depict highly localized strain zones representing two evolving cracks, which initiate at the notch roots. A slight crack curvature can be observed at the bottom crack, and roughly, both cracks can be viewed as straight surfaces with an inclination of about $10^\circ$. In spite of the commented crude representation of the microstructure, the obtained macroscale crack pattern fairly coincides with the results reported in the experiment (Nooru-Mohamed 1992).

Figure 13. Iso-lines of the macroscopic vertical displacements. Grouping of iso-lines indicates a jump in the displacement field and, therefore, signals the crack path

The series of snapshots in Figure 14 show the evolution of the strain injected embedded weak discontinuity region (finite elements in dark grey), and the finite elements with injected embedded strong discontinuities (in red). The weak discontinuity region spreads across a wide zone, forming a bulb-like zone at the tip of each crack endowed with highly
flexible elements, suitable to capture localized strains and their propagation. On this basis, the crack-path-field technique in BOX 3-1, supplies the crack-path, as the zero level set of the crack path field \( \mu_t \), which, in turn, defines the proper position (in every \( \Gamma_t \)-crossed element) of the injected strong discontinuity mode.

Figure 14. Evolution of injected weak discontinuity region (in dark grey), zero-level set of the crack path field (lines in blue) and finite elements injected with strong discontinuity (in red).

Figure 15 displays additional results of the numerical solution. The crack path obtained at the end of analysis is shown in Figure 15-(a), which is compared with the experimental one. The structural response in terms of vertical loads vs. vertical displacement of the top specimen is shown in Figure 15-(b).

Figure 15. Characterization of the structural response. (a) Numerical and experimental crack path; (b) Axial force \( P \) as a function of the axial displacement \( \delta \).
Classical effects of a propagating crack on the structural response are displayed by the softening character of the structural response curve in spite of the very crude representation of the material through the failure cell.

Next, attention is focused on the behavior of the mesoscopic cell at the singular Gauss point, \( \mathbf{x}^{(e)}_{\text{sing}} \) (the one capturing the mesoscopic failure, see Figure 23, and Table 3 in Appendix II) for different elements at the micro-scale. Figure 16 depicts a zoom of the left notch, showing the crack-path (line in blue) and the normal vector, \( \mathbf{n}^{(e)} \), used for embedding the strong discontinuity kinematics in each finite element (see Figure 25, in Appendix II). A number of elements have been selected to analyze the mesoscopic results. For every selected element, the corresponding deformed failure cell, at the end of analysis, is shown. There, it can be checked that those elements crossed by the crack path display a clear mesoscopic failure mode characterized by a (regularized) displacement jump, in a set of cohesive elements, which is constant for all of them as predicted by the theoretical results (see REMARK 2-4). The one down-left the notch, though nearby the crack path, is not crossed by it and, as expected, displays a smooth deformation mode.

![Figure 16. Deformed (amplified) failure cells, for several elements at the macroscale at the end of the analysis, displaying the activated failure mechanism (in red).](image)

4.2.4 Macro-/meso-scale relationship

The effects of distribution and richness of possible failure mechanisms at the mesoscopic cell, and their effects, on the crack patterns at the macro-scale and on the structural response, are now examined.

For this purpose, the original cell in Figure 12-(b) is considered, together with two additional failure cells (see Figure 17). They keep the original material morphology, in terms of matrix and inclusions, but considerably reduce the number of possible failure mechanisms (by locking the inelastic behaviour of appropriated cohesive bands).
Figure 17. Mesoscale cells with different cohesive-band patterns. (a) Original failure cell; (b) Failure cell allowing only a quasi-horizontal failure mechanism; (c) Failure cell allowing an oblique failure mechanism.

In case of Figure 17-(b) the only possible failure mechanism is almost horizontal, whereas in Figure 17-(c), it is oblique.

Figure 18 displays the macroscopic crack pattern obtained with each of these cells.

Figure 18. Crack paths simulated according with the adopted mesoscopic cell.

Figure 19 plots the structural responses in terms of load vs. vertical displacement, provided by the three cells in Figure 17. As it can be expected, locking of failure modes due to removal of cohesive bands at the mesoscopic scale leads to the following response: the poorer is the mesoscopic cell description the higher is the structural strength.
5 Concluding remarks

Along this work, a new approach to two-scale modeling of material failure, based on computational homogenization (FE2), has been presented. The specific features of the approach rely on two main aspects: a) the adopted continuum setting for representation of the fracture, based on the Continuum Strong Discontinuity Approach (CSDA) and developed by the authors in previous works (Oliver, Huespe et al. 2002), and, b) a standard (continuum) format of the computational homogenization procedure.

The resulting framework is endowed with the following properties:

1) Minimally invasive nature with regard to procedures well established in the literature on multiscale modelling of materials. In fact,
   • in terms of the computational homogenization procedure: the proposed approach displays no substantial difference with respect to the ones used for smooth (continuous) problems. A RVE/failure cell is defined at the lower (micro/meso scale) from which stresses and strains are homogenized in a classical continuum format to obtain a, point-wise defined, stress-strain constitutive model at the macro-scale.
   • In terms of material failure propagation: existing algorithms for mono-scale crack propagation modelling can be easily extended to the multi-scale case. In this sense, the authors’ experience in extending the crack-path-field and strain injection techniques (Oliver, Dias et al. 2014) previously developed for the mono-scale case to the present multiscale case, should be extensible to other families of crack-propagation techniques.

2) Objectivity character (independence) of the results in terms of:
   • finite element mesh size and bias, at the macro-scale
   • failure-cell (size and shape) at the micro/meso-scale
Both properties have been assessed in this work through numerical experiments. A key issue in their achievement is the use of an internal/characteristic length, which naturally emerges from theoretical considerations on the homogenized constitutive model, to regularize the weak/strong discontinuity kinematics at the macro-scale in the context of the CSDA.

The performance of the proposed approach has been assessed by a number of examples. They go beyond the, simple, homogenization-based assessment (focusing only on the obtained homogenized macro-scale constitutive equation), but towards a much more ambitious goal: modelling the fracture onset and propagation at the macro-scale based on the, simpler in the physics but more complex in the morphology, micro-scale representations, and the corresponding structural action-response.

However, the authors are aware that realistic multiscale representations of material failure require the use of more sophisticated microscopic morphologies, allowing complex failure mechanisms at the micro-scale (Roubin, Vallade et al. 2015). In this sense, realistic multiscale analysis of material failure, including the extension to 3D cases, face a great challenge: the enormous involved computational cost. It is well known that the algorithmic complexity of multiscale analysis leads to the so-called tyranny of the scales, which make the computations unaffordable, even by resorting to intensive computation procedures, relatively crude representations of the material morphology and coarse finite element meshes at the macro-scale. A possible remedy for this drawback could stem from the development and use of high performance reduced order modelling (HPROM) techniques for multiscale problems. In a recent work (Hernandez, Oliver et al. 2014) the authors have developed some specific and very efficient algorithms for the smooth (continuous) case. Extension to the, much more challenging, non-smooth cases as multiscale material failure, is a subject of ongoing research.

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REFERENCES


Appendix I

Removal of spurious failure modes

When the fundamental localized solution is perturbed, in terms of the micro-fluctuations in equation (21)-(a), by increments
\[ \hat{u}^*_\mu(y) = \mathcal{H}_{\mu}^\text{loc}(y)\hat{\beta}^*_\mu(y) ; \quad \hat{u}^*_\mu(y) \in \mathcal{V}_\mu^* \] (62)
(see equation (16)), \( \hat{\beta}^*_\mu(y,t) \) fulfilling
\[ \hat{\beta}^*_\mu(y) = 0 \quad \text{for some} \quad y \in S_\mu \quad \text{(a)} \]
\[ \hat{\epsilon}^{(i)}(x,t) = \frac{1}{\ell^*_\mu} (\hat{\beta}^*_\mu(x,y) \otimes^\ast n_\mu(x,y)) |_{S_\mu} = 0 \quad \text{(b)} \] (63)
a bifurcation in the solution space \( \sigma - \epsilon \), may appear. Indeed, in this case, the fundamental branch is characterized by the rate equation (see equation (29)-(a)):
\[ \sigma^{(1)}(x,t) = \mathcal{C} : [\hat{\epsilon}(x,t) + \hat{\chi}^*(x,t)] = \mathcal{C}^\text{tang}_{\text{hom}} : \hat{\epsilon}(x,t) \] (64)
On the other hand, the perturbed solution, \( \sigma^{(2)}(x,t) \), is characterized by equations (63); therefore, \( \hat{\epsilon}^{(i)}(x,t) = 0 \) so that substitution in equation (29)-(a) yields:
\[ \sigma^{(2)}(x,t) = \mathcal{C} : (\hat{\epsilon}(x,t) + \hat{\chi}^*(x,t)) \] \[ = \mathcal{C} : [I + \mathcal{M}(\mathcal{E})] : \hat{\epsilon}(x,t) = \mathcal{C}^\ast_{\text{hom}} : \hat{\epsilon}(x,t) \] (65)
Therefore, the fundamental and perturbed solutions in equations (64) and (65) are characterized by different tangent moduli, \( \mathcal{C}^\text{tang}_{\text{hom}} \neq \mathcal{C}^\ast_{\text{hom}} \) (see Figure 20-(a)).
Typically, this situation arises when the perturbation, \( \mathbf{u}_p^*(y) \) in equation (62), consists of a rigid body motion of \( B_p^+ \) with respect to \( B_p^- \) (see Figure 20-(b)) i.e.:

\[
\mathbf{u}_p^*(y) = \mathcal{H}_{B_p}(a + \mathbf{\Omega}(\mathbf{\theta}) \cdot y) \in V_p
\]

(66)

where \( a(t) \) stands for a, spatially constant, shift and \( \mathbf{\Omega}(\mathbf{\theta}(t)) \) is a, skew-symmetric, rotation tensor with axial vector \( \mathbf{\theta}(t) \). From equations (16) and (66):

\[
\int_{\Gamma_p} (\dot{\mathbf{u}}_p^* \otimes \nu_p)^S d\Gamma = \int_{\Omega_p} \mathbf{\nabla} \otimes^S \ddot{\mathbf{u}}_p^*(y,t) d\Omega_p = \\
= \int_{\Omega_p} \mathcal{H}_{B_p}(\mathbf{\Omega} + \mathbf{\Omega}^T) d\Omega_p + \int_{S_p(x)} \mathbf{n}_p(y) \otimes^S (a + \mathbf{\Omega}(\mathbf{\theta}) \cdot y) dS_p = 0
\]

(67)

Equation (67) is a homogeneous system of linear equations in the unknowns \( \{a, \mathbf{\theta}\} \), which can be written as:

\[
\int_{S_p(x)} \mathbf{n}_p(y) dS_p \otimes^S a - \int_{S_p(x)} (\mathbf{n}_p(y) \otimes^S y) dS_p \times \mathbf{\theta} = 0 \rightarrow (a)
\]

\[
- \mathbf{r}(S_p) \otimes^S a + \mathbf{L}(S_p) \times \mathbf{\theta} = 0 \quad (b)
\]

(68)

which can be rephrased as:

\[
\begin{bmatrix} \mathbf{G}(S_p) \end{bmatrix} [a, \mathbf{\theta}]^T = \{0\}
\]

(69)

where \( \begin{bmatrix} \mathbf{G}(S_p) \end{bmatrix} \) is the corresponding matrix of coefficients, depending on the corresponding activated failure mechanism \( S_p \). If \( \begin{bmatrix} \mathbf{G}(S_p) \end{bmatrix} \) is rank deficient, equation (69) has non-trivial solutions, \( \mathbf{a}^*, \mathbf{\theta}^* \), each one characterizing an unstable mode \( \dot{\mathbf{u}}_p^*(y) \) in equation(66). Inspection of equation (68) reveals that if the rotation angle is imposed to be zero \( (\mathbf{\theta} = 0) \) then, the equation becomes

\[
\begin{cases}
\mathbf{r}(S_p) \otimes^S a = 0 \\
\mathbf{r}(S_p) = \int_{S_p(x)} \mathbf{n}_p(y)dS_p = 0
\end{cases} \Rightarrow a = 0
\]

(70)

and system (69) possesses only the trivial solution \( \mathbf{a}^* = 0, \mathbf{\theta}^* = 0 \). This result is exploited in the proposed technique to remove those modes described next.
Consistently with the fundamental result in REMARK 2-4 \((\hat{\beta}_\mu(x,y,t) = \hat{\beta}_\mu(x,t), \forall t \geq t_B)\)
we impose on a selected set, \(B_{\mu,\text{rest}} = \bigcup_{i=1}^{n_{\text{rest}}} B_{\mu,\text{rest}}^{(i)} \subset B_{\mu,\text{coh}}\), of \(n_{\text{rest}}\) cohesive bands (see Figure 2) the following restriction:
\[
\hat{\beta}_\mu^{(i)}(\eta(y),t) \big|_{y \in B_{\mu,\text{rest}}^{(i)} \subset B_{\mu,\text{rest}}} = \hat{\beta}_\mu^{(i)}(t),
\]
\(i = \{1, \ldots, n_{\text{rest}}\}; \forall t \geq t_B\)
In equation (71) notation \(\|(\eta(\xi,\eta))^{\pm}\| \equiv (\eta(\xi,\eta))_{k} - (\eta(\xi,\eta))_{k=0}\) stands for the apparent jump of \((\eta(\xi,\eta))\) between both sides of the cohesive band, see Figure 2. Restriction in equation (71) translates into clamping (precluding rotation but allowing a constant fluctuation jump) domain \(B_\mu^+\) with respect to domain \(B_\mu^-\), by means of the restriction on the cohesive band \(B_{\mu,\text{coh}}^{(i)}\) (see Figure 20-(c)). This is enough to remove the instability modes for any failure mechanism containing the cohesive band \(B_{\mu,\text{coh}}^{(i)}\) \(^{11}\).
Moreover, for practical purposes, and due to the small bandwidth \(k\) of the bands, equation (64) is imposed at the beginning of the analysis, and in total (non-rate) form, without substantial consequences in the results, i.e.:
\[
\hat{\beta}_\mu^{(i)}(\eta(y),t) \big|_{y \in B_{\mu,\text{rest}}^{(i)} \subset B_{\mu,\text{rest}}}^{\pm} = \hat{\beta}_\mu^{(i)}(t),
\]
\(i = \{1, \ldots, n_{\text{rest}}\}; \forall t\)
In this context, it can be readily proven that if any activated failure mechanism contains, at least, one of the cohesive bands of set \(B_{\mu,\text{rest}}\) in equation (72), than equation (52)-(b) has only the trivial solution \(\hat{\beta}_\mu(y) = 0\) and the instability does not appear. From the authors’ experience, to prevent instabilities for any possible failure mechanism it is sufficient to include in the set \(B_{\mu,\text{rest}}\) all cohesive bands intersecting the boundary of the failure cell \(B_\mu\) \(^{12}\).
As for the implementation of equation (72), the restriction can be strongly imposed, as an internal constraint in the elemental nodes, or weakly imposed via a penalty formulation. From the authors’ experience, results are the same for both cases, though the second method turns out to be less code-invasive than the first one.

**Appendix II**

**Strain injection techniques in multiscale problems**

1. **Weak discontinuity injection. Constant stress/discontinuous strain mode.**

1.1 **Dipole generalized function**

Let us denote \(\chi_{\delta^+}(x)\) as the dipole generalized function (generalized derivative of the Dirac’s delta function) fulfilling

11 If quadrilateral finite elements are used for modeling the cohesive bands, equation (69) is equivalent to impose the fluctuation jump \([\hat{\beta}_\mu^+(\xi,\eta)(y_j,t)]^+\) to be the same for all nodes, \(j\), placed in the \(\eta\) direction of the selected element (see Figure 5).

12 The fact that any failure mechanism intersects the boundary of the failure cell is exploited for this statement.
\[ \int_B \chi_{S^*} \phi(x) dB = \int_{S^*} [\phi] dS \]  
(73)

for any sufficiently regular function, \( \phi(x) \) exhibiting a jump, \([\phi]\), across the discontinuity path, \( S^* \). Let us also define a two-parameter \((h,k)\) sequence, \( \chi_{S^*}^{h,k}(x) \), in a band of thickness \( \ell \) as:

\[
\chi_{S^*}^{h,k}(x) = \begin{cases} 
- \frac{1}{h-k} & x \in B_{\text{reg}} \\
\frac{1}{k} & x \in B_{\text{sing}} \\
0 & \text{otherwise}
\end{cases}
\]  
(74)

which is sketched, for the 2D case, in Figure 21. It can be readily checked that \( \chi_{S^*}^{h,k}(x) \) fulfills equation (73) in the limit \( h \to 0 \), \( k \to 0 \), so that it can be considered a regularized sequence converging to the dipole function in equation (73).

![Figure 21. Regularized dipole function \( \chi_{S^*}^{h,k} \).](image)

A very important property of the regularized dipole function \( \chi_{S^*}^{h,k}(x) \), to be exploited for subsequent purposes, is (see Figure 21),

\[ \int_B \chi_{S^*}^{h,k} dB = 0 \]  
(75)

1.2 Injection of a constant-stress/discontinuous-strain mode in quadrilateral elements

Let us consider the microscopic instantaneous density of dissipation, \( \mathcal{D}_m(y,t) \), at the micro-scale:

\[ \mathcal{D}_m(y,t) := \sigma \cdot \dot{\epsilon}_m - \psi \geq 0 \]  
(76)

where \( \psi(y,t) \) stands for the microscopic free energy density of the corresponding constitutive model. From equation (76), and taking into account the Mandel-Hill equation (17), the macroscopic instantaneous density of dissipation, \( \mathcal{D}(x,t) \), can be written as:

\[
\mathcal{D}(x,t) := \frac{1}{\Omega_m} \int_{\Omega_m} \mathcal{D}_m(y,t) dV = \sigma : \dot{\epsilon} - \psi \geq 0 \quad (a)
\]

\[
\psi(x,t) := \frac{1}{\Omega_m} \int_{\Omega_m} \psi_m(y,t) dV \quad (b)
\]

where \( \psi(x,t) \) is defined, through equation (77)-(b), as the averaged (macroscopic) density of free energy, \( \psi_m \), at the microscale.
Then, considering a finite element discretization of the domain, \( B \), in quadrilateral elements, \( B(\varepsilon) \); \( B = \bigcup_{e=1}^{n_{elem}} B^{(e)} \), the injection domain, \( B_{inj} \), is defined as
\[
B_{inj}(t) := \{ \bigcup_{e} B^{(e)} ; \ \mathcal{D}(x_{\varepsilon}^{(e)}, t) > 0 \}
\]
(78)
where \( x_{\varepsilon}^{(e)} \) stands for the barycenter of element \( (e) \). Equation (78) defines \( B_{inj}(t) \) as the locus, at time \( t \), of the elements of the macroscale experiencing inelastic behavior at the corresponding microscale level (evaluated at their barycenter \( x_{\varepsilon}^{(e)} \)). A subset of the injection domain, the weak discontinuity domain \( B_{wd}(t) \) is now defined as:
\[
B_{wd}(t) := \{ \bigcup_{e} B^{(e)} ; B^{(e)} \subset B_{inj}(t) ; t \leq t_B(x_{\varepsilon}^{(e)}) \}
\]
(79)
Equation (79) characterizes \( B_{wd}(t) \) as the set of elements of the injection domain \( B_{inj}(t) \) whose barycenter has not yet bifurcated, according to the definition of the bifurcation time, \( t_B \), in equation (37).

The points of \( B_{wd} \) are now endowed a weak discontinuity kinematics, by resorting to the assumed enhanced strain concept ((Simo and Rifai 1990a; Simo and Oliver 1994)). The rate of strain, injected in rate form at the typical element, \( e \), with \( n_{node} \) nodes, is the following:
\[
\dot{\varepsilon}^{(e)}(x, t) \equiv \dot{\varepsilon}_{i}^{(e)}(x) = \sum_{i=1}^{n_{node}} \nabla N_i(x) \otimes \dot{d}_i(t) + \frac{\chi_{S}^{(e)} \ell_{\varepsilon}^{(e)}(x) \dot{\varphi}^{(e)}(t)}{\alpha^{(e)}(x) \in \mathcal{B}^{(e)} \subset B_{wd}(t)}
\]
(80)
where \( N_i \) are the standard shape functions, \( \dot{d}_i(t) \), the nodal displacements, and \( \chi_{S}^{(e)} \ell_{\varepsilon}^{(e)} \) is the element “\( e \)” counterpart of the regularized dipole-function in equation (74), for:
\[
k \equiv \ell_{\mu}^{(e)} = \ell_{\mu}(x_{\varepsilon}^{(e)})
\]
fufilling (see Figure 22):
\[
\chi_{S}^{(e)} \ell_{\varepsilon}^{(e)}(x) = \begin{cases} 
\frac{1}{h^{(e)} - \ell_{\mu}^{(e)}} & x \in B_{reg}^{(e)} \\
\frac{1}{\ell_{\mu}^{(e)}} & x \in B_{sing}^{(e)} \\
0 & \text{otherwise}
\end{cases}
\]
(81)
where \( h^{(e)} \) is a characteristic element width, defined in terms of the measure (area/volume) of the element, \( \Omega^{(e)} \), and the measure (length/area), \( L^{(e)} \), of the element crack path \( S^{(e)} \).

Notice that, by construction, the element dipole function, \( \chi_{S}^{(e)} \ell_{\varepsilon}^{(e)} \), defined in equation (81) fulfills, at element level, the condition in equation (75), i.e.:
Figure 22. Injected weak discontinuity mode. Elemental regularized dipole function $\chi^{\delta^{(e)}\mu^{(e)}}_S$.

The second term in equation (80) injects, by means of the mode $\chi^{\delta^{(e)}\mu^{(e)}}_S$, a discontinuous strain field, intensified by the elemental strains $\dot{\gamma}^{(e)}(t)$.

Notice that equation (80) can be rewritten as

$$
\dot{\varepsilon}^{(e)}(x) = \sum_{i=1}^{i=n_{node}} \nabla N_i(x) \otimes^s \dot{d}_i(t) + \dot{\gamma}^{(e)}(x) \equiv \tilde{\dot{\gamma}}^{(e)}(x) = \chi^{\delta^{(e)}\mu^{(e)}}_S (x) \tilde{\gamma}^{(e)}(x)
$$

where the enhanced strains, $\tilde{\gamma}^{(e)}(x)$, fulfill (in view of equation (75)) the condition:

$$
\int_{\hat{B}^{(e)}} \tilde{\gamma}^{(e)}(x) = 0 \quad \forall \hat{B}^{(e)}
$$

this defining a specific class of assumed-enhanced strain elements (Simo and Rifai 1990a). Notice also the role of the internal length $\ell^{(e)}_\mu = \ell^{(e)}_{\mu}(x^{(e)}_B)$, imported from the lower scale at the element barycenter, in the definition in equations (81) and (83), in accordance with REMARK 2-3.

A subsequent refinement of the weak discontinuity injection in equation (80) consists of the sub-integration, at the element barycenter, of the first term of the right-hand-side of equations (83). This can be interpreted as a complemental injection of an element-wise constant strain field for describing the compatible-strains part in equation (73). The resulting mixed finite-element problem in BOX 3-2 can be solved in closed form, resulting (Oliver, Huespe et al. 2010):

$$
\dot{\varepsilon}^{(e)}(x) = \sum_{i=1}^{i=n_{node}} \phi^{(e)}(x^{(e)}_B) \otimes^s \dot{d}_i(t) + \dot{\gamma}^{(e)}(x,t)
$$

where $\phi^{(e)}(x)$ is the characteristic function of element $e$ ($\phi^{(e)}(x) = 1 \quad \forall x \in B^{(e)}$, $\phi^{(e)}(x,t) = 0 \quad \forall x \not\in B^{(e)}$).
It is well known that, for the considered quadrilateral elements, sub-integration of the compatible strains, may translate into violation of the inf-sup conditions (Zienkiewicz and Taylor 1994) and the subsequent appearance of zero-energy modes polluting the solution (hour-glass modes). However, it has to be emphasized that, in equation (85) reduced integration is restricted to just a portion of the whole domain (the weak discontinuity domain $B_{wd}(t) \subset B$ defined in equation (79)). This dramatically changes, in a favorable sense, the stability properties of the resulting formulation. The possible hourglass modes do not appear whenever a sufficient portion of the domain is fully integrated (Oliver, Dias et al. 2014).

**BOX 1: Weak-discontinuity injection variational problem (in rate form)**

**PROBLEM**

**GIVEN**:  
\[ l^*_i := \{ \hat{\eta_i}(x) = \sum_{e=1}^{n_{elem}} N_e(x) \eta_e \in [H^1(B)]^{n_{dim}} ; \eta_e(x)_{|_{\partial B}} = \hat{u}_i^*(x,t) \} \]
\[ l^*_0 := \{ \eta(x) \in H^1(B) ; \eta(x)_{|_{\partial B}} = 0 \} \]
\[ \delta\hat{\mu} := \sum_{e=1}^{n_{elem}} \delta \mu^{(e)}(x) \; \delta \mu^{(e)} ; \delta \mu^{(e)} \in \mathbb{S}^{n_{dim} \times n_{dim}} \}
\[ \hat{\Gamma} := \{ \delta \hat{\gamma} = \sum_{e=1}^{n_{elem}} \chi_{S}^{(e)} \delta \hat{\gamma}^{(e)} ; \delta \hat{\gamma}^{(e)} \in \mathbb{S}^{n_{dim} \times n_{dim}} \} \]

**FIND**:  
\[ \hat{u}_i(x) \equiv \hat{u}(x,t) : B \times [0,T] \to \mathbb{R}^{n_{dim}} ; \hat{u}_i \in l^*_i \]
\[ \hat{\epsilon}_i(x) \equiv \hat{\epsilon}(x,t) : B \times [0,T] \to \mathbb{S}^{n_{dim} \times n_{dim}} ; \hat{\epsilon}_i \in \hat{\epsilon} \]
\[ \hat{\gamma}_i(x) \equiv \hat{\gamma}(x,t) : B \times [0,T] \to \mathbb{S}^{n_{dim} \times n_{dim}} ; \hat{\gamma}_i \in \hat{\gamma} \]

**FULFILLING**:  
\[ \int_B \nabla^* \eta : \dot{\sigma}_i \; d\mathcal{B} - W^{ext}(\eta, \dot{\eta}, \dot{b}, \dot{t}^*) = 0 \quad \forall \eta \in l^*_0 \quad (a) \]
\[ \int_B \delta \mu : (\hat{\epsilon}_i - \nabla^S \hat{u}_i(x)) d\mathcal{B} = 0 \quad \forall \delta \mu \in \hat{\epsilon} \]
\[ \hat{\epsilon}_i(x,t) = \hat{\epsilon}_i(x) + \hat{\gamma}_i(x) \]
\[ \hat{\epsilon}_i(x) = \sum_{e=1}^{n_{elem}} \phi^{(e)}(x) \; \hat{\epsilon}_i^{(e)} \rightarrow \text{assumed (regular) strain} \quad (b) \]
\[ \hat{\gamma}_i(x) = \sum_{e=1}^{n_{elem}} \chi_{S}^{(e)} \hat{\gamma}_i^{(e)}(x) \; \hat{\gamma}_i^{(e)} \in \hat{\gamma} \rightarrow \text{enhanced (singular) strain} \]
\[ \int_B \delta \hat{\gamma} : \dot{\sigma}_i d\mathcal{B} = \sum_{e=1}^{n_{elem}} \delta \hat{\gamma}^{(e)} \int_{B^{(e)}} \chi_{S}^{(e)} \hat{\gamma}_i^{(e)}(x) : \dot{\sigma}_i^{(e)} d\mathcal{B} = \]
\[ = \sum_{e=1}^{n_{elem}} \int_{S^{(e)}} \delta \hat{\gamma}^{(e)} : [\dot{\sigma}_i]_{S^{(e)}} d\Gamma = 0 \quad \forall \delta \hat{\gamma}^{(e)} \in \mathbb{S}^{n_{dim} \times n_{dim}} \]
\[ \dot{\sigma}_i(x,t) \equiv \dot{\sigma}_i(x) = \Sigma(\hat{\gamma}_i(x)) \rightarrow \text{constitutive equation} \quad (d) \]

The resulting injection procedure is summarized in BOX 1. It provides a finite element formulation, highly sensitive to propagation of localized strain fields. In spite that the actual kinematics of a strong discontinuity, fulfilling equation (3), is not included, and, therefore, some degree of stress locking could still appear (Oliver, Huespe et al. 2012) the resulting
element provides reliable information for the crack path field problem in BOX 3-1. Therefore, it is used as a first ingredient of the proposed crack-propagation algorithm.

1.3 Stress sampling and integration rule

The standard (four) Gauss quadrature rule, corresponding to full integration of two-dimensional quads, is complemented with two additional sampling points (placed at the center of the element), see Figure 22 and Figure 23. They are termed the singular sampling point, denoted \( x_{\text{sing}}^{(e)} \), and the regular sampling point, denoted \( x_{\text{reg}}^{(e)} \) and sampling the rest of the element. Entities to be sampled (typically the stresses) are then additionally stored at these additional sampling points as it is done for regular sampling points.

Therefore, for the weak-discontinuity injected element, numerical integration (typically, evaluation of the incremental internal forces in terms of the stresses), is based on those two injection-sampling points, by defining the weights indicated in Table 3:

Table 3: Sampling values for the regularized dipole function, \( \chi_{S}^{h^{(e)}, \varepsilon_{\mu}^{(e)}} \), Dirac’s delta function \( \delta_{S}^{(e)} \), and integration weights at the injection sampling points.

<table>
<thead>
<tr>
<th>Sampling point</th>
<th>Sampling value ( \chi_{S}^{h^{(e)}, \varepsilon_{\mu}^{(e)}} )</th>
<th>Sampling value ( \delta_{S}^{(e)} )</th>
<th>Weight</th>
</tr>
</thead>
</table>
| **Regular s.p.:** \( x_{\text{reg}}^{(e)} \) | \[
-\frac{1}{h^{(e)} - \varepsilon_{\mu}^{(e)}} \]
\[
h^{(e)} = \frac{\Omega^{(e)} - L^{(e)}}{\varepsilon_{\mu}^{(e)}}
\] | 0 | \( \Omega^{(e)} - \varepsilon_{\mu}^{(e)} L^{(e)} \) |
| **Singular s.p.:** \( x_{\text{sing}}^{(e)} \) | \( \frac{1}{\varepsilon_{\mu}^{(e)}} \) | \( \frac{1}{\varepsilon_{\mu}^{(e)}} \) | \( \frac{1}{\varepsilon_{\mu}^{(e)}} L^{(e)} \) |

Figure 23. Sampling points involved in the numerical integration.

Replacement of the integration rule, in Table 3, into equation (87)-(b)-(c) yields the element-wise equation.
where $\Sigma_{\text{sing}}$ and $\Sigma_{\text{reg}}$ stand for the stress-evaluation via the continuum constitutive model at the regular and singular sampling points, respectively, as stated by the continuum strong discontinuity approach. Typically, $\Sigma_{\text{sing}}$ is made inelastic with strain softening (the softening modulus is regularized with the internal length, $\ell_\mu$), and $\Sigma_{\text{reg}}$ is enforced to be instantaneously elastic (for both loading and unloading).

Equation (88)-(b) states that the (incremental) stress field is constant all over the element, in spite of the imposed discontinuous strain field in Figure 22. In addition, equation (88)-(c) supplies an elementary-uncoupled additional equation for solving the strain jump, $\hat{\gamma}_i^{(e)}$, in terms of the regular elemental strain, $\hat{\varepsilon}_i^{(e)}$. Therefore, the additional degrees of freedom, $\hat{\gamma}_i^{(e)}$, corresponding to the enhanced strain can be condensed at element level following standard procedures (Simo and Rifai 1990b; Oliver 1996b; Dolbow and Devan 2004).

2. Injection of a propagating strong discontinuity

In a second stage, a propagating strong discontinuity is injected in the following domain:

$$B_{\text{sd}}(t) := \{ \bigcup_\varepsilon B^{(e)} ; \; B^{(e)} \subset B_{\text{reg}}(t) \; ; \; t > t_B(x^{(e)}) \} \quad (89)$$

Comparing equations (89), (78) and (79) one realizes that the strong discontinuity injection takes place as soon as a weak-discontinuity-injected element bifurcates according to the problem in equation (36). In other words, as soon as the homogenized strain field at the upper scale is compatible with a strong discontinuity kinematics (see equations (36) and (39)).

Let us now consider the continuum body, $B$, (see Figure 24-(a)) split by the strong discontinuity path $S$ into two parts, $B^+$ and $B^-$. Across $S$, the rate of displacement field, $\dot{\mathbf{u}}(\mathbf{x})$, experiences a jump $[\dot{\mathbf{u}}] = \dot{\mathbf{u}}|_{k \in (\partial B^+ \cap S)} - \dot{\mathbf{u}}|_{k \in (\partial B^- \cap S)}$.

![Figure 24. (a) Body exhibiting a strong discontinuity. (b) Strong discontinuity kinematics. (c) Unit jump function.](image-url)
The kinematic description of the displacement field in $\mathcal{B}$, (see Figure 24-(a)) reads:

$$\dot{\mathbf{u}} = \mathbf{u} + \mathcal{H}_S [\dot{\mathbf{u}}]$$  \hspace{2cm} (90)

where $\dot{\mathbf{u}}$ stands for the smooth part of the displacement field, $\dot{\mathbf{u}} \equiv \dot{\mathbf{u}}|_{\mathbf{x} \in (\partial \mathcal{B}^r \cap \mathcal{S})} - \dot{\mathbf{u}}|_{\mathbf{x} \in (\partial \mathcal{B}^s \cap \mathcal{S})}$ stands for the displacement jump and $\mathcal{H}_S$ is the Heaviside (step) function, shifted to $\mathcal{S}$. Due to computational reasons, related to the imposition of the essential boundary conditions, it is convenient to re-formulate equation (90) as the following equivalent expression, see (Oliver 2000) for further details,

$$\dot{\mathbf{u}} = \dot{\mathbf{u}} - \varphi[\dot{\mathbf{u}}] + \mathcal{H}_S[\dot{\mathbf{u}}] = \dot{\mathbf{u}} + \frac{(\mathcal{H}_S - \varphi)[\dot{\mathbf{u}}]}{\mathcal{M}_S}$$  \hspace{2cm} (91)

where $\dot{\mathbf{u}}$ fulfills the Dirichlet boundary conditions of the problem, $\varphi$ is a continuous, in principle arbitrary, function fulfilling:

$$\varphi(\mathbf{x}) = \begin{cases} 0 & \forall \mathbf{x} \in (\mathcal{B} \setminus \mathcal{B}_M) \setminus \mathcal{S} \\ 1 & \forall \mathbf{x} \in (\mathcal{B} \setminus \mathcal{B}_M) \cap \mathcal{S} \end{cases}$$  \hspace{2cm} (92)

In equation (92) $\mathcal{M}_S(\mathbf{x}) = \mathcal{H}_S - \varphi(\mathbf{x})$ is the unit jump function, whose support is $\mathcal{B}_M$ and exhibits a unit jump across $\mathcal{S}$, see Figure 24. In equation (92), $\varphi(\mathbf{x})$ is the so-called indicatrix function (Oliver, Dias et al. 2014). The (infinitesimal) strain field corresponding to equation (91) reads:

$$\dot{\varepsilon} = \nabla^\mathcal{S}\dot{\mathbf{u}} = \nabla^\mathcal{S}\dot{\mathbf{u}} + (\mathcal{M}_S \otimes \nabla^\mathcal{S}\dot{\mathbf{u}})^S - (\nabla \varphi \otimes \dot{\mathbf{u}})^S + \delta^\mathcal{S}(\mathbf{n} \otimes \dot{\mathbf{u}})^S = \dot{\varepsilon} + \delta^\mathcal{S}(\mathbf{n} \otimes \dot{\mathbf{u}})^S$$  \hspace{2cm} (93)

In the present multiscale context, the proposed injection procedure consists of the incremental injection of the elemental strong discontinuity mode,

$$\dot{\varepsilon}^{(e)} = \begin{cases} \dot{\varepsilon}^{(e)}(t) + \dot{\gamma}^{(e)}(\mathbf{x},t) & \forall \mathcal{B}^{(e)} \in \mathcal{B}_{sd}(t) \\ \text{(regular, constant, strains)} & \text{(singular, enhanced strains)} \end{cases}$$  \hspace{2cm} (94)

$$\dot{\varepsilon}^{(e)}(t) = \sum_{i=i}^{\mathcal{I}} \nabla N_i(x_i^{(e)}) \otimes \dot{d}_i(t)$$

$$\dot{\gamma}^{(e)}(\mathbf{x},t) = \delta^\mathcal{S}_S(\dot{\mathbf{f}}^{(e)}(\mathbf{x}) \otimes \mathbf{n}^{(e)}(\mathbf{x}))$$

in terms of the $\dot{\mathbf{f}}^{(e)(e)}$-regularized Dirac’s delta function, $\dot{\varepsilon}^{(e)}$, displayed in Figure 25, and Table 3, fulfilling

$$\delta^\mathcal{S}_S = \begin{cases} 1 & \mathbf{x} \in \mathcal{B}^{(e)}_{\text{sing}} \\ 0 & \mathbf{x} \in \mathcal{B}^{(e)}_{\text{reg}} \end{cases}$$  \hspace{2cm} (95)
Figure 25. Injected strong discontinuity mode. Elemental regularized Dirac’s
delta function $\delta_{S}^{(e)}$.

Notice the directional, and placement-dependent, character of the injected mode in
equations (94)-(95) and Figure 25, in contrast with the isotropic weak-discontinuity mode in
equations (85) and Figure 22. Precise information of this placement, ensuring the spatial
continuity of the injected crack-path is a fundamental requirement in the method. The
direction of the element normal, $\mathbf{n}^{(e)}$, is provided by the solution, $\mathbf{n}$, of the discontinuous
bifurcation problem in equation (37), evaluated at the center of the element $\mathbf{x}^{(e)}$ and at the
bifurcation time $t_{B}(\mathbf{x}^{(e)})$. The resulting injection procedure is summarized in BOX 2. The
integration rule is the one displayed in Table 3 and Figure 23.

BOX 2 : Strong-discontinuity injection variational problem (in rate form)

**PROBLEM**

*GIVEN* :

$\hat{l}^{(e)} := \{ \mathbf{u}(x) = \sum_{i=1}^{N_{\text{node}}} N_{i}(x) \mathbf{u}_{i} \in \left[ H^{1}(B) \right]^{n_{\text{dim}}} ; \mathbf{u}(x)|_{\partial B} = \hat{\mathbf{u}}^{*}(x,t) \}$  

$\hat{l}_{0}^{(e)} := \{ \mathbf{u}(x) \in H^{1}(B) ; \mathbf{u}(x)|_{\partial B} = \mathbf{0} \}$  

$\mathbf{\hat{\epsilon}} := \{ \delta \mathbf{u} = \sum_{e=1}^{n_{\text{elem}}} \delta \mathbf{u}^{(e)}(x) \delta \mathbf{u}^{(e)} ; \delta \mathbf{u}^{(e)} \in \mathbb{S}^{n_{\text{dim}} \times n_{\text{dim}}} \}$  

$\mathbf{\hat{\Gamma}} := \{ \delta \mathbf{\gamma} = \sum_{e=1}^{n_{\text{elem}}} \delta \mathbf{\gamma}^{(e)}(x) (\delta \mathbf{\beta}^{(e)} \otimes S \mathbf{n}^{(e)} ; \delta \mathbf{\beta}^{(e)} \in \mathbb{R}^{n_{\text{dim}}} \}$  

*FIND* :

$\mathbf{\hat{u}}_{t}(x) \equiv \hat{\mathbf{u}}(x,t) : B \times [0,T] \rightarrow \mathbb{R}^{n_{\text{dim}}} ; \hat{\mathbf{u}}_{t} \in \hat{\mathbf{l}}^{(e)}$  

$\mathbf{\hat{v}}(x) \equiv \hat{\mathbf{v}}(x,t) : B \times [0,T] \rightarrow \mathbb{S}^{n_{\text{dim}} \times n_{\text{dim}}} ; \hat{\mathbf{v}} \in \hat{\mathbf{\epsilon}}$  

$\mathbf{\hat{\beta}}(x) \equiv \hat{\mathbf{\beta}}(x,t) : B \times [0,T] \rightarrow \mathbb{R}^{n_{\text{dim}}} ; \hat{\mathbf{\beta}} \in \hat{\mathbf{\Gamma}}$
FULFILLING:

\[
\int_{\mathcal{B}} \nabla \eta \cdot \sigma_t \, d\mathcal{B} - W^{\text{ext}}(\eta, \dot{\mathbf{b}}, \mathbf{i}^*) = 0 \quad \forall \eta \in \hat{\mathcal{B}}_0
\]  

(a)

\[
\int_{\mathcal{B}} \delta \mathbf{m} : [\nabla \varepsilon (\mathbf{x}) - (\nabla \phi (\mathbf{x}) \otimes^T \dot{\mathbf{b}}_t (\mathbf{x}))] \, d\mathcal{B} = 0 \quad \forall \delta \mathbf{m} \in \hat{\mathcal{E}}
\]

\[
\dot{\mathbf{e}}_t (\mathbf{x}, t) = \dot{\mathbf{e}}_t (\mathbf{x}) + \dot{\mathbf{y}}_t (\mathbf{x})
\]

(b)

\[
\begin{cases}
\dot{\mathbf{e}}_t (\mathbf{x}) = \sum_{\mathcal{B}^{(c)}(z) \subset \mathcal{B}_{\text{wd}}} \phi^{(c)} (\mathbf{x}) \dot{\mathbf{e}}^{(c)}_t (\mathbf{x}) & \text{assumed (regular) strain} \\
\dot{\mathbf{y}}_t (\mathbf{x}) = \sum_{\mathcal{B}^{(c)}(z) \subset \mathcal{B}_{\text{sd}}} \delta^{(c)} (\dot{\mathbf{y}}^{(c)} (\mathbf{S}) \otimes^S \mathbf{n}^{(c)} (\mathbf{x})) (\mathbf{x}) \in \hat{\Gamma} & \text{assumed (singular) strain}
\end{cases}
\]  

(97)

\[
\int_{\mathcal{B}} (\delta \mathbf{\beta} \otimes^S \mathbf{n}^{(c)}) : \mathbf{X}^{h,f} \cdot \sigma_t \, d\mathcal{B} = \sum_{e=1}^{n_{\text{elem}}} (\delta \mathbf{\beta}^{(c)} \otimes^S \mathbf{n}^{(c)}) : \int_{\mathcal{S}^{(c)}} \mathbf{X}^{h,f} (\mathbf{x}) \sigma_t^{(e)} (\mathbf{x}) \, d\Gamma = 0 \quad \forall \delta \mathbf{\beta}^{(c)} \in \mathbb{R}^{n_{\text{dim}}}
\]

\[
\sigma (\mathbf{x}, t) \equiv \sigma_t (\mathbf{x}) = \Sigma (\dot{\mathbf{e}}_t (\mathbf{x})) \rightarrow \text{constitutive equation}
\]

3. Space and time integration

As commented above, injection of weak-discontinuity and strong-discontinuity modes, in sections 1 and 2, requires, in principle, specific integration rules in space, i.e.: a standard four-point Gauss quadrature rule, \( \mathbf{x}_i, \ i = (1, 2, 3, 4) \), in \( \mathcal{B} \setminus \mathcal{B}_{\text{nj}} (t) \), and the two additional sampling/injection points, \( \mathbf{x}_{\text{sing}}^{(c)} \) and \( \mathbf{x}_{\text{reg}}^{(c)} \), for injected elements, \( \mathcal{B}^{(c)} \subset \mathcal{B}_{\text{wd}} (t) \) and \( \mathcal{B}^{(c)} \subset \mathcal{B}_{\text{sd}} (t) \) so that \( \mathcal{B}_{\text{nj}} = \mathcal{B}_{\text{wd}} \cup \mathcal{B}_{\text{sd}} \) (see Table 3, Figure 21 and Figure 22).

This domain-specific integration rule can become cumbersome in two senses:

1) Domains \( \mathcal{B} \setminus \mathcal{B}_{\text{nj}} (t) \), \( \mathcal{B}_{\text{wd}} (t) \) and \( \mathcal{B}_{\text{sd}} (t) \) change with time (see Figure 26). This poses, in principle, some additional problems on the time-integration of the resulting rate of the mechanical balance of forces.

2) The implementation of those specific integration rules in a standard finite element code becomes code-invasive.

Figure 26. Evolution of the injection domains for three typical stages of the discontinuity propagation (\( t_1 < t_2 < t_3 \)).
These flaws can be readily overcome by the following procedure. After standard manipulations, the discrete (finite element) version of problem in equations (59)-(a), (87)-(a) and (97)-(a) reads:

\[
\begin{align*}
\mathbf{R}_{\text{mech}}(\mathbf{d}(t)) &= \int_{\mathcal{B}_{\text{inj}}(t)} \mathbf{B}^T(x) \cdot \{ \mathbf{\sigma}(x, \mathbf{d}(t)) \} d\mathcal{B} + \\
&\quad + \int_{\mathcal{B}_{\text{wd}}(t)} \mathbf{B}^T(x) \cdot \{ \mathbf{\sigma}(x, \mathbf{d}(t)) \} d\mathcal{B} + \\
&\quad \int_{\mathcal{B}_{\text{sd}}(t)} \mathbf{B}^T(x) \cdot \{ \mathbf{\sigma}(x, \mathbf{d}(t)) \} d\mathcal{B} - \mathbf{F}^{\text{ext}}(t) = 0
\end{align*}
\]

where, \( \mathbf{R}_{\text{mech}}(\mathbf{d}(t)) \) stands for the mechanical residue (unbalanced forces), \( \mathbf{d}(t) \) is the vector of nodal displacements, \( \mathbf{B}^T(x) \) stands for the classical deformation matrix, \( \{ \mathbf{\sigma}^h(x, \mathbf{d}(t)) \} \) are the homogenized stresses (in Voigt's notation) computed in accordance with the corresponding strain injections and \( \mathbf{F}^{\text{ext}} \) are the external forces. Notice that, dependence on time of the integration domains, \( \mathcal{B}_{\text{inj}}(t), \mathcal{B}_{\text{wd}}(t) \) and \( \mathcal{B}_{\text{sd}}(t) \), in equation (98), makes time integration of the residue equation \( (\mathbf{R}(t); t \in [0, t_{n+1}] \rightarrow \mathbf{R}(t_{n+1}) = 0) \) a sensitive issue.
BOX 3: Effective stress evaluation.

DATA: $\phi_{n+1}(\mathbf{x}), \Delta \hat{u}_{n+1}(\mathbf{x}), \Delta \beta_{n+1}^{(e)}, \sigma_{n+1}^{(e)}(\mathbf{x}), \sigma_{n}^{(e)}(\mathbf{x}), \mathcal{B}_{ad}(t_{n+1}), \mathcal{B}_{ad}(t_{n+1})$

OUTPUT: $\sigma_{n+1}^{(e)}(\mathbf{x}), \sigma_{n}^{(e)}(\mathbf{x})$

1) Compute the elemental indicatrix function:

$$\phi_{n+1}(\mathbf{x}) \rightarrow \phi_{n+1}^{(e)}(\mathbf{x}) = \sum_{i=1}^{n_{\text{node}}} N_i(\mathbf{x}) \phi_i^{(e)}(\phi_{n+1})$$

2) Compute strains, $\varepsilon_{n+1}^{(e)}$, at all sampling points

$$\varepsilon_{n+1}^{(e)}(\mathbf{x}_i) = \varepsilon_{n}^{(e)}(\mathbf{x}_i) + \Delta \varepsilon_{n+1}^{(e)}(\mathbf{x}_i), \quad \mathbf{x}_i \equiv \mathbf{x}_{G_i} \quad (i = 1, \ldots, 4), \mathbf{x}_{\text{reg}}, \mathbf{x}_{\text{sing}}$$

$$\Delta \varepsilon_{n+1}^{(e)}(\mathbf{x}_{\text{reg}}) = \left\{ \begin{array}{ll}
\nabla^{S} \Delta \hat{u}_{n+1}(\mathbf{x}_{\text{reg}}) & B^{(e)} \subset B \setminus (B_{ad} \cup B_{ad})(t_{n+1}) \\
\nabla^{S} \Delta \hat{u}_{n+1}(\mathbf{x}_{\text{reg}}) + \chi_{S}^{(e)} \mathbf{j}_{n}^{(e)}(\mathbf{x}_{\text{reg}}) \Delta \gamma_{n+1}^{(e)} & B^{(e)} \subset B_{ad}(t_{n+1}) \\
\nabla^{S} \Delta \hat{u}_{n+1}(\mathbf{x}_{\text{reg}}) - (\nabla_{\text{sing}}^{(e)}(\mathbf{x}_{\text{reg}}) \otimes \Delta \beta_{n+1}^{(e)})^{S} & B^{(e)} \subset B_{ad}(t_{n+1})
\end{array} \right.$$

$$\Delta \varepsilon_{n+1}^{(e)}(\mathbf{x}_{\text{sing}}) = \left\{ \begin{array}{ll}
\nabla^{S} \Delta \hat{u}_{n+1}(\mathbf{x}_{\text{sing}}) & B^{(e)} \subset B \setminus (B_{ad} \cup B_{ad})(t_{n+1}) \\
\nabla^{S} \Delta \hat{u}_{n+1}(\mathbf{x}_{\text{sing}}) + \chi_{S}^{(e)} \mathbf{j}_{n}^{(e)}(\mathbf{x}_{\text{sing}}) \Delta \gamma_{n+1}^{(e)} & B^{(e)} \subset B_{ad}(t_{n+1}) \\
\nabla^{S} \Delta \hat{u}_{n+1}(\mathbf{x}_{\text{sing}}) + \left[ \frac{\nabla^{(e)}(\mathbf{x}_{\text{sing}})}{h^{(e)}} \right] \otimes \Delta \beta_{n+1}^{(e)} & B^{(e)} \subset B_{ad}(t_{n+1})
\end{array} \right.$$

3) Compute regular stresses, $\sigma_{n+1}^{(e)}$, at all sampling points

$$\sigma_{n+1}^{(e)}(\mathbf{x}_i) = \Sigma[\varepsilon_{n+1}^{(e)}(\mathbf{x}_i)], \quad \mathbf{x}_i \equiv \mathbf{x}_{G_i} \quad (i = 1, \ldots, 4)$$

$$\sigma_{n+1}^{(e)}(\mathbf{x}_{\text{reg}}) = \Sigma_{\text{reg}}[\varepsilon_{n+1}^{(e)}(\mathbf{x}_{\text{reg}})]$$

$$\sigma_{n+1}^{(e)}(\mathbf{x}_{\text{sing}}) = \Sigma_{\text{sing}}[\varepsilon_{n+1}^{(e)}(\mathbf{x}_{\text{sing}})]$$

4) Update effective stresses, $\sigma_{n+1}^{(e)}$, at standard (Gauss) sampling points $\rightarrow \mathbf{x}_i \equiv \mathbf{x}_{G_i} \quad (i = 1, \ldots, 4)$

$$\sigma_{n+1}^{(e)}(\mathbf{x}_i) = \sigma_{n}^{(e)}(\mathbf{x}_i) + \Delta \sigma_{n+1}^{(e)}(\mathbf{x}_i)$$

$$\Delta \sigma_{n+1}^{(e)}(\mathbf{x}_i) = \left\{ \begin{array}{ll}
\sigma_{n+1}^{(e)}(\mathbf{x}_i) - \sigma_{n}^{(e)}(\mathbf{x}_i) & B^{(e)} \subset B \setminus (B_{ad} \cup B_{ad})(t_{n+1}) \\
\sigma_{n+1}^{(e)}(\mathbf{x}_{\text{reg}}) - \sigma_{n}^{(e)}(\mathbf{x}_{\text{reg}}) & B^{(e)} \subset B_{ad}(t_{n+1}) \\
\xi [\sigma_{n+1}^{(e)}(\mathbf{x}_{\text{sing}}) - \sigma_{n}^{(e)}(\mathbf{x}_{\text{sing}})] + \\
+(1-\xi)[\sigma_{n+1}^{(e)}(\mathbf{x}_{\text{reg}}) - \sigma_{n}^{(e)}(\mathbf{x}_{\text{reg}})] & B^{(e)} \subset B_{ad}(t_{n+1})
\end{array} \right.$$

$$\xi = \frac{h^{(e)}}{h^{(e)}}$$

However, this issue can be easily solved by appropriately rephrasing the integral kernels in equation (98). In (Oliver, Dias et al. 2014) it is proven that, by defining some specific stress entities (the so called effective stresses, $\bar{\sigma}(\mathbf{x}, t)$) at the standard Gauss points, the spatial integration in equation (98) can be rephrased to a standard four Gauss points integration rule in the whole integration domain $B$ (and, therefore, not time dependent) i.e.

$$\mathbf{R}_{\text{mech}}(t) \equiv \mathbf{R}_{\text{mech}, t} = \int_{B} B^{T} \left( \mathbf{x} \right) \cdot \left\{ \dot{\mathbf{r}}(\mathbf{x}, \mathbf{d}(t)) \right\} d\mathbf{B} - \mathbf{F}^{\text{ext}}(t) = 0 \quad (99)$$
Now, equation (99) can be exactly integrated\(^{13}\) along the time interval \([0,t_{n+1}]\) as:

\[
R_{\text{mech}}(d_{n+1}) = \int_B B^T(x) \cdot \left\{ \tilde{\sigma}_{n+1}(x,d_{n+1}) \right\} dB - F^{\text{ext}}(t)
\]

\[
= \sum_{\forall B^{(e)} \subset B} \int_{B^{(e)}} B^{(e)T}(x) \cdot \left\{ \tilde{\sigma}_{n+1}^{(e)}(x) \right\} dB - F^{\text{ext}}_{n+1} = 0
\]

(100)

which returns the classical format for the unbalanced residual forces at the current time \(t_{n+1}\). The specific rules for updating the effective stresses, \(\tilde{\sigma}_{n+1}^{(e)}\) appearing in equation (100), in terms of the homogenized stresses, \(\tilde{\sigma}_{n+1}\) at all sampling points, are given in BOX 3.

4. Staggered resolution of the coupled propagation-injection problem

The crack-path-field problem defined in BOX 3-1 is stated in terms of \(\alpha(x,t)\) (the localized strain-like internal variable, which depends directly on the solution, nodal displacements, \(d_{n+1}\), of the non-linear mechanical problem in equation (100). On the other hand, this mechanical problem also depends on the crack path, \(\mu(x,t)\), obtained from the crack path field problem in BOX 3-1 (see Figure 27).

Thus, both problems are coupled, and two sets of discretized, in time and space, equations can be written in terms of the corresponding residues:

\[
R_{\text{mech}}(d_{n+1},\mu_{n+1}) = 0, \quad (a)
\]

\[
R_{\text{prop}}(d_{n+1},\mu_{n+1}) = 0, \quad (b)
\]

(101)

where \(R_{\text{prop}}\) stands for the residue of the crack propagation problem\(^{14}\) in BOX 3-1 and \(\mu_{n+1}\) is the vector of nodal values of the crack-path field \(\mu(x,t_{n+1})\).

As for the strain injection procedure, it can be noticed that, at the initial stages of the non-linear loading process \(B^{\text{inj}} = \emptyset\), no discontinuity is injected and, therefore, the problem in equation (101) is uncoupled in the sense propagation-problem →

\(^{13}\) Assuming zero initial balanced forces.

\(^{14}\) which, unlike the mechanical problem, can be proven to be a linear problem.
mechanical-problem. In this case equation (101)-(a) can be first directly solved for $d_{n+1}$ and then, equation (101)-(b) can be solved for $\mu_{n+1}$:

$$R_{\text{mech}}(d_{n+1}) = 0 \rightarrow d_{n+1} \quad (a)$$
$$R_{\text{prop}}(d_{n+1}, \mu_{n+1}) = R_{\text{prop}}^*(\mu_{n+1}) = 0 \rightarrow \mu_{n+1} \quad (b)$$

As soon as at least one element belongs to $B_{\text{proj}}$, the problem becomes coupled in both senses.

However, numerical experience shows that this coupling is weak. In fact, the dependence of the mechanical problem on the variable $\mu(x)$ is only through the instantaneous position of the discontinuity path, $S_t$, to determine the indicatrix function $\varphi$ and the sets $B_{\text{proj}}$ (see Figure 27), so that the coupling between $d_{n+1}$ and $\mu_{n+1}$ in the term $R_{\text{mech}}(d_{n+1}, \mu_{n+1})$ can be considered weak. This suggests the use of a staggered simplified procedure, replacing $\mu_{n+1}$ by $\mu_n$ in equation (101)-(a), leading to the set of uncoupled equations

$$R_{\text{mech}}(d_{n+1}, \mu_n) = R_{\text{mech}}^*(d_{n+1}) = 0 \rightarrow d_{n+1} \quad (a)$$
$$R_{\text{prop}}(d_{n+1}, \mu_{n+1}) = R_{\text{prop}}^*(\mu_{n+1}) = 0 \rightarrow \mu_{n+1} \quad (b)$$

The staggered resolution of the coupled problem that leads to the uncoupled equations (103) allows envisaging the crack-path-field problem in BOX 3-1 as a post-processing procedure (typically a double smoothing) of the localizing variable $\alpha_n(x)$ in the mechanical problem. The crack propagation problem can then be interpreted as a local (element-wise based) tracking algorithm that can be straightforwardly, implemented in a finite element code in a non-invasive manner.