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An objective multi-scale model with hybrid injection

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ABSTRACT

This paper presents a new semi-concurrent multi-scale model to study the behaviour of composite materials in softening regime. A mixed formulation is used to simulate discontinuities in both scales. The traction over the crack is included as a unknown field in the equations system of the problem, and the jump displacement across the discontinuity is obtained with a cohesive constitutive relation (traction-separation law).

Axiomatic variational principles and the injection concept are used and formulated to get an objective model with respect to the representative volume element size (**RVE**). The projected stress over the normal vector of the macro discontinuity is injected in the localized domain in the **RVE**, obtaining as a dual variable the jump of the displacement field in the macro structure. In this way, during the stable phase of the behaviour, the scale transition is performed in the classical way injecting the strain tensor and obtaining the stress tensor as a dual variable. At the beginning of the unstable regime, the transition between the scales is defined by injecting the traction (stress projection on the normal vector to the crack) in the localization domain in the micro scale and the displacement jump at the macro scale is obtained as a dual variable. This new concept leads to a new multi-scale approach with an hybrid injection.

The basic equations of the model are derived, and finally some numerical examples are developed, showing the objectivity of the homogenized response of composite material problems that involve strain localization at the macro-scale.

1. Introduction

Multi-scale modelling is a trend research area in the computational mechanics community. This kind of models can be divided in two main groups: Multi-scale models based on *analytic methods* and those based on *computational methods*. Analytic methods can be classified in *continualization* methods and *homogenization* methods. In continualization methods, the micro/meso scale is considered as discrete elements like masses, springs or tribology elements, and Taylor series are used to define the transition to the macro-scale [1,2]. In *homogenization* methods the sub-scale is continuous and heterogeneous, while the macro-scale is continuous and homogeneous and they are normally used to obtain elastic properties at the macro-scale [3–8]. Analytic methods are nowadays being displaced by *computational multi-scale methods* that have greater versatility [9].

Park and Liu [10] and Oden at al. [11] proposed a classification of computational multi-scale modelling *hierarchical* and *concurrent* multi-scale models. Hierarchical approaches are normally used to calibrate constitutive equations while concurrent multi-scale models consider the different constituents of the composite at a lower scale.

Bohm [12] classified methods that couple continuum models in: *mean-field approximation methods* [13–15], *variational bounding methods* [16–18] and *methods based in the representative volume element (**RVE**) concept*. Methods based in the **RVE** concept can be divided in:

– Hierarchical methods: The material is constitutively described in some length scale by using an homogenization of a lower scale. These methods are adequate for materials that require a sequence of scales for their description, like laminated or bio-materials. Although this approach does not consider an unitary cell in its definition, it is used in most of the developed models [19–24]. Another approach that contains this type of hierarchical multi-scale models is that of *quasi-phenomenological* models in which an internal variable is calibrated using the **RVE** concept [25].

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– Semi-concurrent methods: These models insert a primary field (strain, temperature gradient, etc.) as a boundary condition in the **RVE**, relating both scales through a compatibility equation (generally an energy type equation). Once the boundary value problem in the micro-scale is solved, a constitutive tensor and an homogenization operator to obtain the dual variable (stress, thermal flux, etc.) is computed for the macro scale. These models are colloquially known as FE^2 models [26–31].
– Concurrent methods: In this kind of formulations the **RVE** is embedded in the zone of interest within the macro-scale. It has been used to couple continuum and atomic scales, where the fractured region is modelled by broken up inter-atomic forces [32,33]. When both scales are modelled by continuous formulations non-matching meshes can be used, getting the compatibility with Lagrange multipliers. This approach has the disadvantage of being computationally expensive when the length scale of the **RVE** is not close to the macro-scale length [34]. Some authors have used this approach to simulate concrete specimens [31,35].
– Hybrid methods: These methods involve a combination of concurrent and semi-concurrent approaches. Within a localization regime, semi-concurrent models generally become non-objective with respect to the **RVE** size. Hybrid models consider a semi-concurrent formulation for macro-scale zones in stable regime, while in unstable zones where a fracture is propagated or damage progress is spread, the **RVE** is embedded in the macro-structure. Akbari [36] proposed an hybrid multi-scale model for fracture analysis of polycrystallines materials.

During the last decades several sophisticated models based on the **RVE** concept, have been proposed for the simulation of quasi-brittle localization at the macro-scale. A formulation that calibrates damage evolution by using a **RVE** with classical interface elements and is able to model fracture evolution in mode I at the macro-scale, has been proposed by Verhoosel et al. [37]. This approach was latter expanded [38,39] for mixed fracture modes, considering cohesive and adhesive elements. Massart et al. [40] presented a continuous–discontinuous homogenization scheme using a first order computational homogenization (FOCH) with the capability of localizing the strain field in the macro-structure and they used it to study the failure mechanism of masonry. In the field of moderate localizations, a new kind of semi-concurrent multi-scale formulations was proposed by Kouznetsova et al. [41]. The strain gradient is transferred as a rotation on the boundary of the **RVE** arriving to a gradient enhanced method at the macro scale combined with a classical description for the micro-scale. This kind of formulations is known as second order homogenization scheme (SOCH) [42–44].

Some attempts to enhance FOCH models have also been published. A two-scale failure multi-scale model expressed as an expansion of the variational framework presented in [45], was presented by Toro et al. [46] introducing the *injection operator* concept proposed in [47]. The macro-scale jump, modelled using an E-FEM technology, is introduced as a boundary condition in the localized domain of the **RVE**. Analogously to the model proposed in [38], an homogenized traction-separation law is obtained. A similar approach has been developed for the analysis of quasi-brittle fracture processes using cohesive bands technology [48]. In this case, the localization band in the macro-scale is calibrated using a characteristic length obtained in the **RVE** and an objective regularization is achieved with this parameter.

This kind of FOCH enhanced models, represents a trend research area with many challenges. Debonding and matrix fracture phenomena in composites with strongly different stiffness can be analysed with mixed methods, like augmented Lagrangian formulations based on displacement and the crack tension, avoiding ill-conditioning problems associated with penalty methods [49,50]. Classic multiscale approach [45] or two-scale failure multi-scale model presented by Toro et al. [51] cannot be directly used in conjunction with mixed approaches to simulate discontinuities in the micro and macro-scale. A new semi-concurrent multi-scale model based on an hybrid injection, formulated in a consistent variational framework is proposed in this paper to simulate composite material failure. The novelty of this approach is that is obtained as a natural extension of the classic formulation [45] to the case of mixed approaches. The proposed multi-scale model involves a stress–strain description in the stable phase and a traction-separation law for the unstable regime. A classical multi-scale model is used to obtain the strain–stress relationship [45], while when an unstable phase is reached and the material starts a softening regime, a model that links localization in both scales injecting the traction at the macro-scale discontinuity in the RVE is presented. Lagrange multipliers representing tension at the fracture are treated like the kinematic field in the classic approach [45]. In this way the stress injection in the cracks corresponding to the localization domain of the RVE has a clear physical meaning and equations analogous to those obtained in one field approaches [45,46] are obtained. By the other side, it is well recognized that traction based boundary conditions can be more naturally introduced than periodic conditions in the localizing regime. In accordance to this observation, Coenen and co-workers [52,53] proposed the use of so called percolation-path-aligned boundary conditions that consist of a gradual transition from periodicity RVE boundary conditions towards more relaxed boundary conditions when localization is detected.

A mixed formulation based on the displacement and the crack tension, is used to simulate discontinuities in both scales and it is presented in Section 2. The proposed model, based on the axiomatic philosophy proposed in [26,47], is presented in Section 3. Some numerical examples, where the objectivity of the homogenized traction-separation law is shown, are presented in Section 4. Finally, conclusions and future trends in this research area, are drawn in Section 5.

2. Mixed formulation for quasi-brittle fracture simulation. A general background

A method based on a mixed functional that considers as unknown variables the displacement field and the crack traction field is used to simulate the fracture process in both scales. A brief description is presented in this section. More details can be found in [49,54].

2.1. Variational formulation

Let $\mathscr{L}^{\boldsymbol{u}} : \mathscr{U} \rightarrow \boldsymbol{R}$ be a system potential dependent on the displacement field $\boldsymbol{u}$ of a infinitesimally deformable body including a fracture Γ (see Fig. 1), expressed as:

$$\mathscr{L}^{\boldsymbol{u}}(\boldsymbol{u}) = \mathscr{L}^{\mathcal{B}}(\boldsymbol{u}) + \mathscr{L}^{\mathcal{F}}(\llbracket \boldsymbol{u} \rrbracket), \tag{1}$$

where $\llbracket \bullet \rrbracket = (\bullet)|_{\Gamma^+} - (\bullet)|_{\Gamma^-}$ represents the jump of the field $(\bullet)$ over the domain Γ. The potential of the bulk domain $\Omega = \Omega^- \cup \Omega^+$ is denoted with $\mathscr{L}^{\mathcal{B}}$ and $\mathscr{L}^{\mathcal{F}}$ is the fracture potential of the crack in Γ, that are defined as follows:

$$\mathscr{L}^{\mathcal{B}}(\boldsymbol{u}) = \frac{1}{2}\int_{\Omega \setminus \Gamma} \boldsymbol{\sigma}(x,t) : \nabla^s \boldsymbol{u}(x,t)\ d\Omega - \int_{\Omega \setminus \Gamma} \boldsymbol{b}(x) \cdot \boldsymbol{u}(x,t)\ d\Omega$$
$$- \int_{\partial^t \Omega} \boldsymbol{p}(x,t) \cdot \boldsymbol{u}(x,t)\ d\partial^t \Omega \tag{2}$$
$$\mathscr{L}^{\mathcal{F}}(\llbracket \boldsymbol{u} \rrbracket) = \int_{\Gamma} \Psi(\llbracket \boldsymbol{u} \rrbracket, \kappa)\ d\Gamma,$$

being $\boldsymbol{b} \in \mathbf{L}^2(\Omega \setminus \Gamma)$ is the volumetric force, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\nabla^s \boldsymbol{u}$ is the symmetric part of the displacement field gradient. In the Neumann boundary $\partial^t \Omega$ a distributed load $\boldsymbol{p} \in \mathbf{L}^2(\partial^t \Omega)$ is considered. In the Dirichlet boundary $\partial^u \Omega$ a prescribed displacement value $\bar{\boldsymbol{u}}$ is applied. The normal vector to the crack Γ is denoted as $\boldsymbol{n}$. The kinematically admissible set $\mathscr{U}(\Omega \setminus \Gamma)$ is defined as:

$$\mathscr{U}(\Omega \setminus \Gamma) = \{\boldsymbol{u} \in \mathbf{H}^1(\Omega \setminus \Gamma)\ \wedge\ \llbracket \boldsymbol{u} \rrbracket \cdot \boldsymbol{n} \geq 0 \in \mathbf{H}^{\frac{1}{2}}(\Omega) : \boldsymbol{u}|_{\partial^u \Omega} = \bar{\boldsymbol{u}}\}. \tag{3}$$