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AN ADAPTIVE MULTISCALE METHOD FOR FRACTURE BASED ON CONCURRENT - HIERARCHICAL HYBRID MODELLING

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ABSTRACT

In this paper, we present a multiscale method to analyse quasi-brittle crack propagation in metals. The fracture model is described at the grain level by damage mechanics. In order a tractable solution to be obtained by numerical means in an engineering component, the microscale behaviour is upscaled at an engineering scale by classical computational homogenization. The lack of scale separation due to the coalescence of microscopic defects is tackled by a concurrent computation of the process zone. The paper focuses on the tools for such a method to be used in practice. In particular, we investigate the adaptive refinement of the process zone within the hybrid concurrent/homogenization-based multiscale strategy, and the time integration of the resulting multiscale problem by an arc-length method.

1 INTRODUCTION

Multiscale approaches aim at solving problems at the engineering (macro) scale while considering the complexity of the micro structure with minimum cost. By splitting the solution between micro and macro contributions, one upscales the features of the fine scale problem to the macroscale where the solution becomes tractable. The macroscale problem is obtained by averaging the microscale properties over representative volume elements (RVE). When both the macroscale problem and local averages are obtained by finite element, the resulting strategy is called FE^2 in the engineering community [1, 2, 3, 4]. This method suffers from a well-known lack of scale separation when strain localization appears in a representative volume element. In other words, when the balance equations of an RVE lose ellipticity, a statistically representative volume element cannot be identified in this region. Consequently, the average theorem on which FE^2 relies is not valid in the corresponding region. This difficulty is particularly stringent in the case of grain plasticity, which we describe in this contribution by cohesive zone models at the scale of the grains.

We propose to devise an adaptive strategy that alleviates this difficulty. The FE^2 technique is used in the safe regions of the granular structure, where representative volume elements of relatively small size can be defined. In the region where localization appears, a domain decomposition scheme is used to solve the problem exactly at the scale of the material heterogeneities A schematic of the combined concurrent-hierarchical multiscale method is shown in Figure 1.

The present contribution defines the basic tools for such a method to be successfully used in grain plasticity. In particular, we investigate (i) the coupling scheme between hierarchical multiscale modelling and domain decomposition approach (ii) the adaptive identification of the region where localisation happens (ii) the time integration of the quasi-static multiscale problem by a dissipation control.

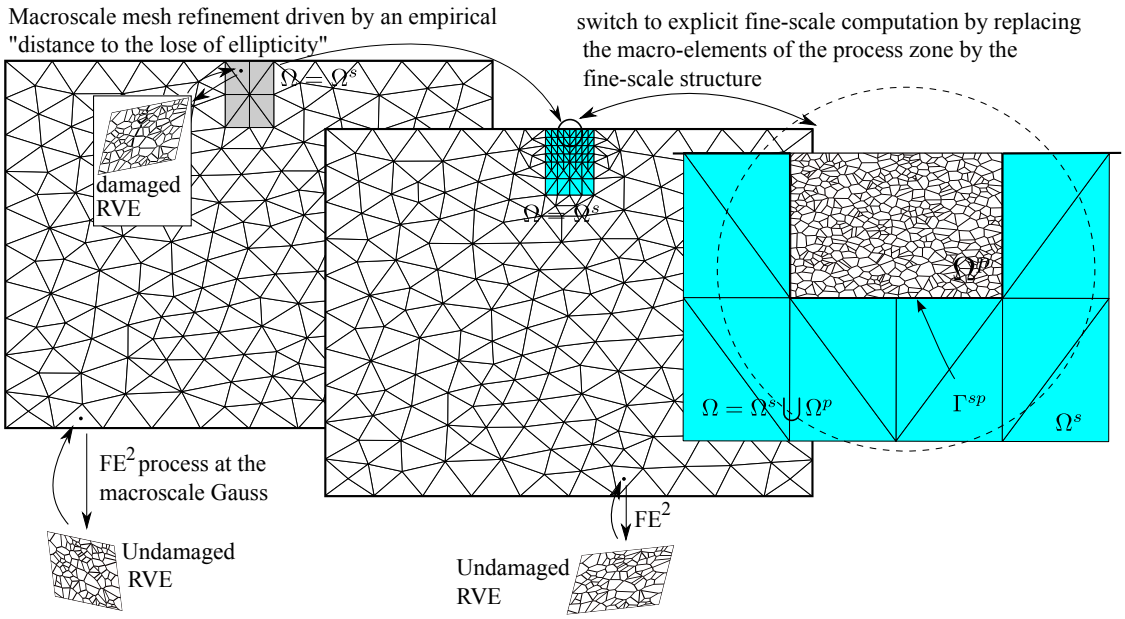

Figure 1: Adaptive hybrid multiscale method

2 HIERARCHICAL / CONCURRENT MULTISCALE METHOD

Microscale problem. Let us consider a domain Ω occupied by a structure consisting of randomly distributed linear orthotropic grains (figure 1) undergoing quasi-static small perturbations. The potential failure of the interface between adjacent grains is described by a cohesive model:

$$\boldsymbol{\sigma}.\mathbf{n} = \mathbb{k}[\![\mathbf{u}]\!] \quad \text{where} \quad \mathbb{k} = \begin{bmatrix} k_n(1-h([\![\mathbf{u}]\!].\mathbf{n})\,d_n) & 0 \\ 0 & k_t(1-d_t) \end{bmatrix}_{(\mathbf{n},\mathbf{t})} \tag{1}$$

where $(\mathbf{n},\mathbf{t})$ is the local basis defined by the normal and tangential unit vectors to the interface between two grains, h is the heaviside step function, k_n and k_t are the normal and tangential stiffness coefficients of the elastic damageable model and d_n and d_t are two damage indicators that range from 0 (safe interface) to 1 (completely damaged). The damage variable are related to the history over time of the jump of displacement $[\![\mathbf{u}]\!]$ in order to represent the irreversible fracture process.

Model-based computational homogenisation proposes to search for an effective displacement field $\mathbf{u}^c \in \mathcal{U}^M(\Omega)$ defined over Ω which satisfies the macroscale variational equilibrium (under the assumption that no volume force is applied to the structure):

$$\int_\Omega \boldsymbol{\sigma}^c : \boldsymbol{\delta\epsilon}^c \, d\Omega = \int_{\partial\Omega_F} \mathbf{F}_d.\boldsymbol{\delta u}^c \, d\Gamma \qquad \forall\, \boldsymbol{\delta u}^c \in \mathcal{U}^{c,0} \tag{2}$$

At arbitrary point $\mathbf{x}^c \in \Omega$, the relationship between the effective stress tensor $\boldsymbol{\sigma}^c$ and the symmetric part of the effective displacement gradient $\boldsymbol{\epsilon}^c = \frac{1}{2}\left(\boldsymbol{\nabla u^c} + (\boldsymbol{\nabla u^c})^T\right)$ is defined via averaging of the microscopic constitutive law over a representative volume element $\theta(\mathbf{x}^c)$:

$$\begin{aligned} \boldsymbol{\epsilon}^c &= \frac{1}{|\theta(\mathbf{x}^c)|}\int_{\partial\theta(\mathbf{x}^c)} \mathbf{u}^f \otimes_s \mathbf{n}\, d\Gamma \qquad && \text{Strain averaging over an RVE} \\ \boldsymbol{\sigma}^c &= \frac{1}{|\theta(\mathbf{x}^c)|}\int_{\partial\theta(\mathbf{x}^c)} \mathbf{t}^f \otimes \mathbf{x}^f\, d\Gamma \qquad && \text{Effective stress tensor} \end{aligned} \tag{3}$$

In the above equations, $\mathbf{u}^f \in \mathcal{U}^f(\theta(\mathbf{x}^c))$ is the microscale displacement field defined over $\theta(\mathbf{x}^c)$, the symmetrised tensor product operator is defined by $\mathbf{u}^f \otimes_s \mathbf{n} = \frac{1}{2}(\mathbf{u}^f \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}^f)$, and $\mathbf{x}^f$ is an arbitrary point of the RVE. The fine-scale boundary traction field $\mathbf{t}^f$ and fine scale displacement $\mathbf{u}^f$ are found by solving the equilibrium and constitutive laws of the microstructure over the RVE, which reads: $\forall\, \boldsymbol{\delta u}^f \in \mathcal{U}^{f,0}(\theta(\mathbf{x}^c))$,

$$\sum_{G\in\mathcal{G}(\theta(\mathbf{x}^c))} \int_G \boldsymbol{\epsilon}^f : \mathbb{H}^{(G)} : \boldsymbol{\delta\epsilon}^f \, d\theta + \sum_{G\in\mathcal{G}(\theta(\mathbf{x}^c))} \frac{1}{2}\int_{\partial G\setminus\partial\theta(\mathbf{x}^c)} \mathbf{t}^{(G)}.[\![\boldsymbol{\delta u}^f]\!]^{(G)}\, d\Gamma = \int_{\partial\theta(\mathbf{x}^c)} \mathbf{t}^f.\boldsymbol{\delta u}^f \, d\Gamma \tag{4}$$

where $\mathcal{G}(\theta(\mathbf{x}^c))$ is the ensemble of domains occupied by individual grains belonging to the RVE, and $\mathbb{H}^{(G)}$ is the Hooke's tensor corresponding to the orthotropic linear behaviour of grain $G \in \mathcal{G}(\theta(\mathbf{x}^c))$. The second term of the equation is the virtual work of the cohesive tractions $\mathbf{t}^{(G)} = \boldsymbol{\sigma}^f.\mathbf{n}^{(G)}$ in the fine scale virtual displacement field. The last term of this equation accounts for the (dualised) boundary conditions applied to RVE. In a strain-driven homogenisation procedure, these conditions are chosen such that (i) the strain averaging in equation (3) is automatically enforced, and (ii) a separation of scale in an energy sense (Hill-Mandel macrohomogeneity condition) is obtained:

$$\int_{\partial\theta(\mathbf{x}^c)} \mathbf{t}^f.\boldsymbol{\delta}\bar{\boldsymbol{u}}\, d\Gamma = 0 \qquad \forall\, \boldsymbol{\delta}\bar{\boldsymbol{u}} \text{ such that } \int_{\partial\theta(\mathbf{x}^c)} \boldsymbol{\delta}\bar{\boldsymbol{u}}^f \otimes_s \mathbf{n}\, d\Gamma = 0 \tag{5}$$

Discretisation The coarse-scale problem is discretised in space by linear finite element. The scale-transition is enforced at each of the quadrature points of the coarse mesh. The grain distribution of the fine-scale problem required to compute the average quantities is generated randomly, and the resulting fine-scale problem is discretised by linear finite element (FE^2). The semi-discrete multiscale problem is solved by a classical time-stepping integration scheme. A Newton algorithm is employed to solve the nonlinear fully discrete system at each step of the time integration algorithm.

Concurrent approach for the solution in the process zone. Domain Ω is partitioned into a safe domain Ω^s and the process zone Ω^p such that $\Omega^s \cup \Omega^p = \Omega$. The FE^2 method is used to solve approximately the grain plasticity problem over Ω^s. A direct solution strategy is used to find the fine scale displacement in Ω^p. The coupled problem reads:

$$\left\{ \begin{array}{l} \displaystyle\int_{\Omega^s} \boldsymbol{\sigma}^c : \boldsymbol{\delta\epsilon}^c\, d\Omega = \int_{\partial\Omega^s_F} \mathbf{F}_d.\boldsymbol{\delta u}^c\, d\Gamma - \int_{\Gamma^{sp}} \boldsymbol{\lambda}^p.\boldsymbol{\delta u}^c\, d\Gamma \\ \displaystyle\sum_{G\in\mathcal{G}^p} \int_G \boldsymbol{\epsilon}^f : \mathbb{H}^{(G)} : \boldsymbol{\delta\epsilon}^f\, d\Omega + \sum_{G\in\mathcal{G}^p} \frac{1}{2} \int_{\partial G\setminus\partial\Omega^p} \mathbf{t}^{(G)}.[\![\boldsymbol{\delta u}^f]\!]^{(G)}\, d\Gamma = \int_{\Gamma^{sp}} \boldsymbol{\lambda}^p.\boldsymbol{\delta u}^f\, d\Gamma \end{array} \right. \tag{6}$$

where we have assumed for simplicity that no Neumann boundary conditions are applied to the process zone. $\mathcal{G}^p$ is the set of domains corresponding to the grains that belong to the process zone. The relationship between $\boldsymbol{\sigma}^c$ and $\boldsymbol{\delta\epsilon}^c$ is obtained implicitly in Ω^s by the computational homogenisation approach. The coupled problem is complemented by a constraint equation for interface $\Gamma^{sp} = \partial\Omega^s \cap \partial\Omega^p$:

$$\int_{\Gamma^{sp}} \left(\boldsymbol{u}^c_{|\partial\Omega^s} - \boldsymbol{u}^f_{|\partial\Omega^p} \right).\boldsymbol{\lambda}^{p\star}\, d\Gamma = 0 \tag{7}$$

The choice of the admissibility space for Lagrange multiplier $\boldsymbol{\lambda}^p$ characterises the transfer of interface fields between the safe domain and the process zone. We choose in this work to look for this field in the trace on the interface of the macroscale finite element space ("zero fluctuation of the traction fields" across the interface).

3 ADAPTIVITY AND SOLUTION SCHEME

Adaptive identification of the process zone. The idea of the refinement process of the hybrid multiscale method is the following. Where needed, the macroscale mesh used in the computational homogenisation strategy is refined, until the size of a macroscale element is of the order of the characteristic size of the RVE. At this stage, a set of surrounding macroelements are defined as the process zone and the corresponding fine-scale problem is solved in a concurrent manner. Both FE^2 refinement strategy and transition from non-concurrent to concurrent approach require to project internal variables onto newly introduced fine-scale granular structures. Doing so, the dissipation and virtual work of the multiscale problem before and after the refinement should be conserved. This is a difficult issue that we are currently investigating. The other difficulty is to find a reliable criterion to drive the adaptivity. We consider three types of criteria of increasing complexities and associated computational costs:

- A local indicator at the micro-level. The value of the local damage indicators in each RVEs can be used to drive the adaptivity. Such an empirical criterion has the advantage to be extremely easy to implement. It however leads to a pessimistic indication of the loss of scale-separation, and consequently to an early refinement of the FE^2 method.

- A macroscale local empirical criterion which measures a "distance" to the loss of ellipticity. We will show some first results based on the use of the condition number of a normalised homogenised tangent operator to drive the refinement process.
- An error estimation based on a solid mathematical background. In [2], the authors proposed an error estimation and adaptivity framework for multiscale methods applied to nonlinear solid mechanics. Our long-term aim is to extend this method to adaptive multiscale fracture mechanics, and use it to validate (or invalidate) the use of empirical but cheaper and mathematically less complex refinement criteria.

Time integration by dissipation-controlled arc-length method. A robust path-following method is developed to follow the globally unstable quasi-static response of the damaged structure in the proposed multiscale framework (see a related work in[5]). Our strategy is essentially an extension of the arc-length method introduced in [6] for time-stepping incremental solution schemes. The amplitude of the external load is constrained to satisfy a condition on the increase of local microscopic quantities such as damage or local energy dissipation. We will show how this idea can be adapted to the hybrid multiscale framework.

4 CONCLUSION

A hybrid hierarchical / concurrent multiscale technique is proposed for the reliable simulation of fracture in heterogeneous materials. We will show that such a strategy is a promising alternative to classical sub-modelling techniques. We will discuss some of our later developments concerning the analysis of the method and the identification of numerical parameters for the transition of scales and adaptivity.

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References

[1] F. Feyel, J.L. Chaboche. FE2 multiscale approach for modelling the elastoviscoplastic behaviour of long ber SiC/Ti composite materials. *Computer Methods in Applied Mechanics and Engineering*. 2000; 183: 309-330.

[2] F. Larsson,K. Runesson. Adaptive Bridging of Scales in Continuum Modeling Based on Error Control, *International Journal for Multiscale Computational Engineering*, 2008; 6: 371-392.

[3] A. Abdulle. The Finite Element Heterogeneous Multiscale Method: a computational strategy for multiscale PDEs. *GAKUTO International Series Math. Sci. Appl.* 2009; 31: 133-181.

[4] Geers, M.G.D., V.G. Kouznetsova, and W.a.M. Brekelmans. Multi-scale computational homogenization: Trends and challenges. *Journal of Computational and Applied Mathematics*. 2010; 234(7): 2175-2182.

[5] O. Allix, P. Kerfriden, P. Gosselet. On the control of the load increments for a proper description of multiple delamination in a domain decomposition framework. *International Journal for Numerical Methods in Engineering*. 2010; 83(11): 1518-1540.

[6] E. Lorentz, P. Badel. A new path-following constraint for strain-softening finite element simulations. *International Journal for Numerical Methods in Engineering*. 2004; 60(2): 499-526.