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High-performance model order reduction techniques in non-linear multiscale fracture problems

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Micro Abstract
In this work presents a strategy to diminish the computational cost of a hierarchical (FE2) multi-scale computational homogenization approach for fracture problems is presented. Focusing on concepts as Reduced Order Modeling (ROM) based on the POD and optimal integration quadrature techniques, a hyper-reduced order modeling (HPROM) method is specifically derived. This model departs from the multi-scale framework developed in (Oliver/2015) for the numerical modeling of failure.

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Introduction

Multiscale modeling appears as an excellent potential setting to account for the physical links between the different lower scale components, within the material (grains, particles, defects, inclusions, etc.), and the overall large scale properties. However, this modeling concept, coined by the scientific community some decades ago, is not yet part of the routinely engineering analysis and design methods. Certainly, and focusing on the specific case of computational homogenization-based multiscale techniques, they can hardly be applied beyond some simple and academic purposes. Reasons for this arise from the multiplicative character of the algorithmic complexity and the corresponding computational cost, for hierarchical micro/macro computations in multiscale analyses. On the other hand, model order reduction (data compression) techniques have become an intensive research field in the computational mechanics community, because of the increasing interest on computational modeling of complex phenomena in large scale multiphysics problems.

This work deals with a combination of both subjects by focusing on the reduced order modeling of computational multiscale modeling of fracturing materials. In this work, the multiscale framework for numerical modeling of structural fracture in heterogeneous quasi-brittle materials, described in [2]. In this work, a number of techniques are combined to optimize the HPROM performance of FE^2 multiscale modeling algorithms for multiscale propagating fracture. They are: (1) A *domain separation* strategy. The RVE is split into the *regular* domain (made of the elastic matrix and possible inclusions) and the *singular* domain (the cohesive bands exhibiting a softening cohesive behavior), (2) The ROM boundary problem for the RVE is formulated in an unconventional manner i.e.: in terms of the strain fluctuations. (3) A specific Reduced Optimal Quadrature (ROQ) is used as a key technique to obtain relevant computational cost reduction from the ROM. The above techniques are combined to provide the proposed HPROM strategy for the RVE, using a standard two-stage (off-line/on-line) strategy.

Generalities of FE^2 method applied to multiscale fracture problems:

This approach is developed under a small strain framework, the equality of internal power at both scales is guaranteed via *Hill-Mandell Macro-Homogeneity* principle. In this approach, the macroscopic constitutive response is proven to be point-wise equivalent to an inelastic law (in an incremental fashion) as a function of the homogenized elastic tangent tensor, $\mathbf{C}^{hom}$, and the incremental homogenized inelastic strain rate $\dot{\boldsymbol{\varepsilon}}^{(i)}$ i.e.:

$$\dot{\boldsymbol{\sigma}} = \mathbf{C}^{hom} : (\dot{\boldsymbol{\varepsilon}}(x) - \dot{\boldsymbol{\varepsilon}}^{(i)}) \qquad \dot{\boldsymbol{\varepsilon}}^{(i)} = \frac{1}{l_\mu}(\mathbf{n} \otimes \dot{\boldsymbol{\beta}}) \tag{1}$$

Where, the inelastic strain component $\dot{\boldsymbol{\varepsilon}}^{(i)}$ is expressed as a function of the homogenized variables taken from the RVE, and represent the average value of the symmetric tensor product between the strong discontinuity normal $\mathbf{n}$, and the rate of displacement jump $\dot{\boldsymbol{\beta}}$ of each cohesive band, belonging to the manifold of the mesoscopic failure mechanism $\mathcal{S}_\mu$, i.e. the mesoscopic crack. In addition, the so-called *material characteristic length* l_μ is defined as the ratio between the measure (volume or area) of the representative volume and the measure (surface or length) of the mesoscopic failure mechanism. The equations that govern the RVE, rephrased in terms of *micro-strain fluctuations*, are the next:

PROBLEM A: Given a macroscale strain $\boldsymbol{\varepsilon}$, and the spaces of kinematically compatible strain fluctuations $\mathcal{U}_\mu^{\tilde{\varepsilon}}$, and admissible strain fluctuations, $\mathcal{V}_\mu^{\tilde{\varepsilon}}$, find $\tilde{\boldsymbol{\varepsilon}}_\mu \in \mathcal{V}_\mu^{\tilde{\varepsilon}}$, being $\boldsymbol{\varepsilon}_\mu = \boldsymbol{\varepsilon} + \tilde{\boldsymbol{\varepsilon}}_\mu$, such that:

$$\int_{\mathcal{B}_\mu} \boldsymbol{\sigma}_\mu(\boldsymbol{\varepsilon}_\mu, d_\mu) : \widehat{\boldsymbol{\varepsilon}}_\mu \, d\mathcal{B} = 0\,; \quad \forall \widehat{\boldsymbol{\varepsilon}}_\mu \in \mathcal{V}_\mu^{\tilde{\varepsilon}} = \mathcal{U}_\mu^{\tilde{\varepsilon}} := \{\tilde{\boldsymbol{\varepsilon}}_\mu \,|\, \int_{\mathcal{B}_\mu} \tilde{\boldsymbol{\varepsilon}}_\mu \, d\mathcal{B}_\mu = \mathbf{0} \quad \text{and} \quad \tilde{\boldsymbol{\varepsilon}}_\mu \in \mathcal{E}_\mu\}; \tag{2}$$

$$\dot{d}_\mu(\boldsymbol{y}, \boldsymbol{\varepsilon}_\mu) = g(\boldsymbol{\varepsilon}_\mu, d_\mu) \quad \text{being} \quad \mathcal{E}_\mu = \{\boldsymbol{\zeta} \in \mathbb{S}^{n_{dim} \times n_{dim}} \quad | \quad e_{mjq} e_{nir} \boldsymbol{\zeta}_{ij,qr} = 0\}$$

PROBLEM A is completely equivalent to the classical equilibrium problem stated in terms of micro-displacement fluctuations, the original displacement fluctuations, $\tilde{\boldsymbol{u}}_\mu$, can be recovered, if necessary for the deformed RVE visualization purposes, through an additional spatial integration of the equation $\tilde{\boldsymbol{\varepsilon}}_\mu = \nabla^s \tilde{\boldsymbol{u}}_\mu$. However, PROBLEM A could be also rephrased as the minimization of the potential of microscale free energy $\Pi(\tilde{\boldsymbol{\varepsilon}}_\mu, \boldsymbol{\lambda})$, in which the boundary conditions can be applied via *Lagrange multipliers*, it can be shown that this format is suitable for reduction purposes.

PROBLEM B (HF): *(RVE saddle point problem)* Given a macro-scale strain $\boldsymbol{\varepsilon}$, find $\tilde{\boldsymbol{\varepsilon}}_\mu$ and $\boldsymbol{\lambda}$ satisfying:

$$(\tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{\varepsilon}, d_\mu), \boldsymbol{\lambda}(\boldsymbol{\varepsilon}, d_\mu)) = \arg\{\min_{\tilde{\boldsymbol{\varepsilon}}_\mu} \max_{\boldsymbol{\lambda} \in \mathbb{S}^{\boldsymbol{n} \times \boldsymbol{n}}} \Pi(\tilde{\boldsymbol{\varepsilon}}_\mu, \boldsymbol{\lambda})\}; \quad \text{such that} \quad \dot{d}_\mu(\boldsymbol{y}, \boldsymbol{\varepsilon}_\mu) = g(\boldsymbol{\varepsilon}_\mu, d_\mu) \tag{3}$$

Model Order Reduction techniques:

The reduction process is divided into two sequential steps. The first step consists of a Galerkin projection, via Proper Orthogonal Decomposition *POD* of the micro-strain fluctuations field, onto a small space (reduced-order space). We seek for a reduced vectorial space of dimension n_ε, with $n_\varepsilon \ll N_g$, for computing the micro-strain fluctuations. This low-dimension space is obtained as the linear expansion of an orthogonal basis of n_ε spatial functions:

$$\tilde{\boldsymbol{\varepsilon}}_\mu(\boldsymbol{y}, t) = \sum_{i=1}^{n_{\boldsymbol{\varepsilon}}} \boldsymbol{\Psi}_i(\boldsymbol{y}) c_i(t) = \boldsymbol{\Psi}(\boldsymbol{y}) \boldsymbol{c}(t) \tag{4}$$

where each element $\boldsymbol{\Psi}_i$, of the basis $[\boldsymbol{\Psi}]$, is recognized as a micro-strain fluctuation mode and the vector of time dependent coefficients $\boldsymbol{c}(t) = [c_1, \ldots, c_{n_\varepsilon}]$ $(\boldsymbol{c} \in \mathbb{R}^{n_\varepsilon})$ represents the amplitude of these modes, the variations of the micro-strain fluctutations are adopted wth an identical

approach to (4). Now, introducing (4) into the PROBLEM B, and after some manipulations, a new model *Reduced Order Model (ROM)* written in terms of the micro-strain reduced basis has been obtained:

PROBLEM C (ROM): Given a macro-scale strain $\boldsymbol{\varepsilon}$, find $\boldsymbol{c} \in \mathbb{R}^{n_\varepsilon}$ and $\boldsymbol{\lambda} \in \mathbb{R}^{n_{\boldsymbol{\sigma}}}$ satisfying:

$$(\boldsymbol{c}(\boldsymbol{\varepsilon}, d_\mu), \boldsymbol{\lambda}(\boldsymbol{\varepsilon}, d_\mu)) = \arg\left\{\min_{\boldsymbol{c}} \max_{\boldsymbol{\lambda} \in \mathbb{S}^{\boldsymbol{n}\times\boldsymbol{n}}} \Pi(\boldsymbol{\Psi}\boldsymbol{c}, \boldsymbol{\lambda})\right\} \quad (5)$$

$$= \arg\left\{\min_{\boldsymbol{c}} \max_{\boldsymbol{\lambda} \in \mathbb{S}^{\boldsymbol{n}\times\boldsymbol{n}}} \int_{\mathcal{B}_\mu} \psi_{\mu[\boldsymbol{\varepsilon}, d_\mu]}(\boldsymbol{\varepsilon} + \boldsymbol{\Psi}\boldsymbol{c})\, d\mathcal{B}_\mu + \boldsymbol{\lambda}^T \left(\int_{\mathcal{B}_\mu} \boldsymbol{\Psi} d\mathcal{B}_\mu\right) \boldsymbol{c}\right\} \quad (6)$$

$$\text{such that:} \quad \dot{d}_\mu(\boldsymbol{y}, \boldsymbol{\varepsilon}_\mu) = g(\boldsymbol{\varepsilon}_\mu, d_\mu)$$

In many cases, it is an accepted fact that, although ROM markedly reduces the number of unknowns in the problem (in the present case, the dimension n_ε of the vector $\boldsymbol{c}$ in Eq. 4), this does not translate into an actual reduction of the computational cost and, consequently, in a problem speedup. Therefore, further actions should be taken. These actions are known in the literature with the term hyper-reduction [1], which gives rise to the HyPer-Reduced Order Model (HPROM), the main goal is to reduce the number of integration points given by the standard Gauss quadrature, by defining a new scheme that efficiently determines optimal integration points and its corresponding weights so that the error in the integration of the reduced model is minimized. More specifically, the integral term involving the free energy $\psi_{\mu[\boldsymbol{\varepsilon}, d_\mu]}$ is evaluated as:

$$\int_{\mathcal{B}_\mu} \psi_{\mu[\boldsymbol{\varepsilon}, d_\mu]}(\boldsymbol{\varepsilon} + \boldsymbol{\Psi}(\boldsymbol{y})\boldsymbol{c})\, d\mathcal{B}_\mu \approx \sum_{j=1}^{Nr} \psi_{\mu[\boldsymbol{\varepsilon}, d_\mu]}(\boldsymbol{\varepsilon} + \boldsymbol{\Psi}(\boldsymbol{z_j})\boldsymbol{c})\omega_j := \int_{\mathcal{B}_\mu}^{*} \psi_{\mu[\boldsymbol{\varepsilon}, d_\mu]}(\boldsymbol{\varepsilon} + \boldsymbol{\Psi}(\boldsymbol{y})\boldsymbol{c})\, d\mathcal{B}_\mu \quad (7)$$

Taking PROBLEM C, Eq. (7) can be utilized to evaluate the derivatives in the optimality condition (Euler equations), yielding the following set of equations, from now on termed HPROM:

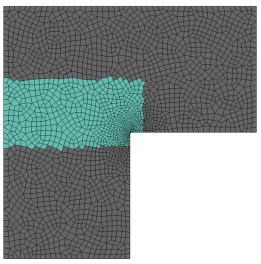
PROBLEM D (HPROM): Given a macro-scale strain $\boldsymbol{\varepsilon}$, find $\boldsymbol{c} \in \mathbb{R}^{n_\varepsilon}$ and $\boldsymbol{\lambda} \in \mathbb{R}^{n_{\boldsymbol{\sigma}}}$ satisfying:

$$\frac{\partial \Pi}{\partial \boldsymbol{c}^T} = \int_{\mathcal{B}_\mu}^{*} \boldsymbol{\Psi}(\boldsymbol{y})\boldsymbol{\sigma}_\mu(\boldsymbol{y}, \boldsymbol{c})\, d\mathcal{B}_\mu + \left(\int_{\mathcal{B}_\mu} \boldsymbol{\Psi}(\boldsymbol{y})^T\, d\mathcal{B}_\mu\right) \boldsymbol{\lambda} = \boldsymbol{0}; \quad \frac{\partial \Pi}{\partial \boldsymbol{\lambda}^T} = \left(\int_{\mathcal{B}_\mu} \boldsymbol{\Psi}(\boldsymbol{y})\, d\mathcal{B}_\mu\right) \boldsymbol{c} = \boldsymbol{0} \quad (8)$$

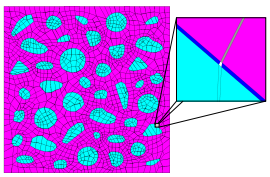
A similar procedure could be also used for the other integral terms in PROBLEM D, but, these being constant terms (not depending on the unknowns of the problem) they can be integrated once for all (presumably in the off-line stage), using the standard Gauss quadrature, the result being stored and used, when necessary, in the on-line stage.

Numerical Results: Application to simulation of fracture in cementitious materials

The macro-scale will be splitted into two subdomains, the dark gray domain will be modeled using an elastic monoscale constitutive law, taking the elastic homogenized constitutive tangent tensor, and, in the green domain the Hiper-Reduced Order Model (HPROM). The finite element mesh of the meso-scale is also depicted in figure (1-b), Material properties have been taken from [3]. The figure (2-a) shows the structural response in terms of load-displacement ($\mathbf{P} - \delta$) curve (vertical load of the bottom, rightmost corner node versus displacement at the same place) for each set of strain modes $n_{\boldsymbol{\varepsilon}}$ and integration points n_r. It is also shown the sensitivity in the convergence of the structural behavior as $n_{\boldsymbol{\varepsilon}}$ increases. In figure (2-b), it can be observed the convergence results for the meso-scale tests using the HPROM; fixing a number of strain modes $n_{\boldsymbol{\varepsilon}}$, we get an optimal number of integration points. In addition, it can be immediately noticed that, as the number of strain modes $n_{\boldsymbol{\varepsilon}}$ increases, the error decreases monotonically. The imposition of a judicious equilibrium between error and number of integration points plays an important role in the good performance of the method.



(a) Macroscale FE discretization



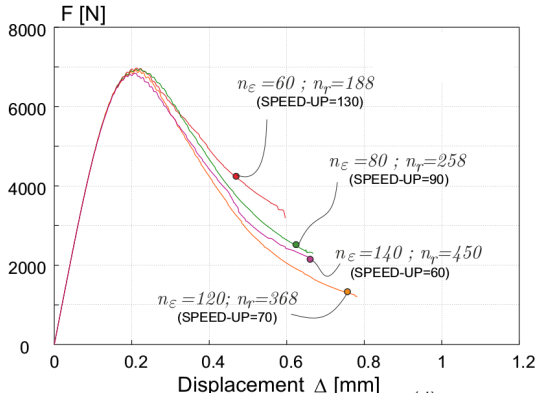
(b) Meso-scale FE discretization

Mortar Matrix			
Young modulus	E_m	[MPa]	18500
Poisson's ratio	ν_m	[-]	0.18
Tensile strength	$f_{t,m}$	[MPa]	2.60
Fracture energy	$G_{f,m}$	[N/m]	140
Aggregates			
Young modulus	E_a	[MPa]	37000
Poisson's ratio	ν_a	[-]	0.18

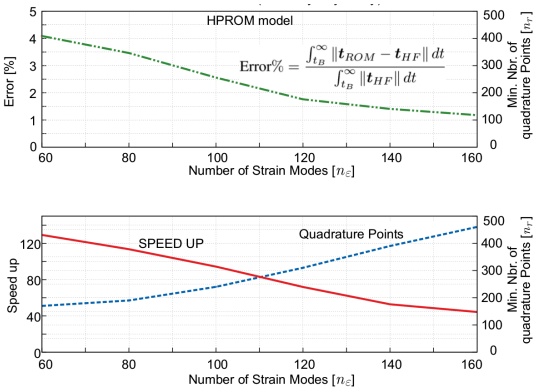
(Unger & Eckard 2011)

(c) Material properties

Figure 1. Finite element discretization and material properties



(a) Macro-structural response - L Shape Panel



(b) Convergence analysis of the meso-scale

Figure 2. Convergence error in macro and meso scales

Conclusions

The result of this work is a reduced model based on a hierarchical FE^2 multiscale approach for material failure in cementitious materials, that preserves all features of the standard FE model [2]. Furthermore, the two presented simulations show the convergence of the meso-scale and the sensitivity of the macro-structural behavior, as a function of the amount of strain modes, $n_{\boldsymbol{\varepsilon}}$, and the number of integration points, n_r. The reduced model solves the problem of unafordable computational cost.

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