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MULTISCALE CONCRETE FAILURE ANALYSIS WITH VIRTUAL ELEMENTS AND INTERFACES

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Abstract. The use of multiscale schemes for computational failure evaluations of composites materials has become a promising topic for evaluating the complex degradation mechanisms at different scales of observations and to achieve accurate information on the effects of these subscales degradation processes on the macroscopic response behavior. In the framework of standard finite element procedures, both concurrent and semi-concurrent multiscale procedures were considered so far for analyzing failure behavior of quasi-brittle materials.

When it comes to composite materials such as concrete, which are characterized by inclusions or aggregates that are strongly heterogeneous with respect to size and geometry, it is absolutely necessary to take into account the mesoscopic scale, since it seriously affects the macroscopic response behavior. However, there are well-founded questions about the capabilities of standard finite element procedures to represent heterogeneous mesoscopic structures such as concrete, because they impose geometric constraints and unrealistic boundary conditions that distort the resulting numerical solutions.

In this work a new approach is pursued for mesoscale analysis of concrete failure behavior. This is based on combining Virtual Elements (VE) and interfaces in the framework of the discrete approach. In the first part of this work, the basis of the VE technology and of the considered interface model are outlined. Then, the procedure for concrete-mesoscopic meshing proposed in this work based on combining VEM and non-linear interface elements (IE) is detailed. Finally, numerical analysis are presented involving stress paths and failure behavior that shows the potential and efficiency of the approach based on VE and IE for composite materials like concrete are discussed.

1 Introduction

In the last decades, mesoscale analysis of cement-based materials became a propitious approach for numerical modeling and failure prediction. The capabilities and precision of the mesoscale analysis depend on the accurate description of the geometry of that scale, and the correct description of the non-linear behavior of the material when submitted to external actions.

Several theoretical models and numerical tools have been proposed with the aim to realistically predict the pre- and post-cracking behavior of concrete at mesoscale levels. In this work a new approach is pursued for thermodynamically consistent [1, 2] analysis of multiscale concrete failure behavior involving mesoscopic RVE. This is based on combining Virtual Elements (VE) [3–6] and interfaces in the framework of the discrete approach. VE allow discretizations of the domain into arbitrary polygons providing effective and realistic approximations of the concrete large and medium size aggregates while the fracture energy-based interfaces facilitate the development of discrete cracks through aggregate-mortar and mortar-to-mortar joints during the monotonic loading procedures.

VEM is a novel development that allows the use of polytopal meshes, and offers a much higher degree of freedom than FEM meshes. It was inspired by techniques used in the Mimetic Differences Method [7] but later was given a framework as a generalization of the standard FEM. VEM meshes have many interesting possibilities such as allowing hanging nodes, improving adaptivity, simple insertion of cracks and fractures as well as facilitating the meshing of complex geometries. For example, whenever independently obtained meshes need to be compatibilized, these simply merge into a globally conforming mesh by sharing all nodes on the common boundary. See for example Fig. 1, where the biggest inclusion is a 70 node rectangle embedded in a fine mesh matrix.

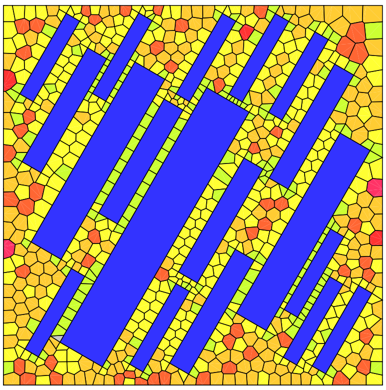

Figure 1: Matrix with inclusion.

As with all new developments, the VEM literature is still in its early stages, specially in experimental results, although it has been steadily growing since its introduction. On the other hand, the method is free from many of the most common disadvantages of other approaches for polygonal meshes and it has been shown to be robust when dealing with highly irregular meshes as well as relatively easy to implement.

Zero-thickness interface elements [8], formulated in terms of contact stresses versus opening relationships, have been historically employed for modeling material discontinuities, i.e. mechanical contacts, bond phenommena, and crack evolutions in quasi-brittle materials like concrete. Several plasticity-based interface formulations have been proposed to predict failure behaviors of discontinuities in soil/rock mechanisms. One of the most frequent use of interface elements in computational concrete mechanics is related to mesoscopic failure simulations.

The mathematical formulation of VEM as a generalization of standard FEM for (even nonconvex) polyhedra is described in Section 2. Then, the basic equations behind the use of zero-thickness interface elements is given in Section 3. Section 4 summarizes the meshing procedure for describing the composite nature of concrete. Section 5 exemplifies this procedure for a three point bending notched concrete beam. Finally, some concluding remarks are reported in Section 6.

2 The Virtual Element Method for Mechanical problem

2.1 Formulation for Mechanical problem

The problem is to find displacements $\mathbf{u} : \Omega \to \mathbb{R}^d$, such that

$$\begin{cases} -\boldsymbol{\nabla}\cdot\boldsymbol{\sigma} & = \mathbf{f} \quad \text{in } \Omega \\ \mathbf{u} & = 0 \quad \text{on } \Gamma_D \\ \boldsymbol{\sigma}\cdot\mathbf{n} & = 0 \quad \text{on } \Gamma_N \end{cases} \tag{1}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress, $\mathbf{f}$ the body forces, $\mathbf{n}$ is the outward-pointing normal; and Γ_D and Γ_N are the Dirichlet and Neumann boundaries respectively.

Considering the strain $\boldsymbol{\varepsilon} = \boldsymbol{\nabla}^s\mathbf{u}$, and the constitutive relation $\boldsymbol{\sigma} = \boldsymbol{E} : \boldsymbol{\varepsilon}$ (being $\boldsymbol{E}$ the mechanical material operator), the variational form of the problem is then to find an allowable displacement $\mathbf{u}$ such that

$$a(\mathbf{u},\mathbf{v}) = \int_\Omega \mathbf{f}\cdot\mathbf{v}\, d\Omega \tag{2}$$

with

$$a(\mathbf{u},\mathbf{v}) = \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{u}) : \boldsymbol{E} : \boldsymbol{\varepsilon}(\boldsymbol{v})\, d\Omega\,. \tag{3}$$

2.2 The Virtual Element Method

In short, the VEM is a generalization of standard FEM to meshes made up by arbitrary, possibly non-convex polyhedra. It was first introduced in [9] and the basic ideas are recalled here for the case of the general second order elliptic equation (described in [10]).

A summary of the VEM numerical procedure will be given in this section. For more details see [11].

Discretization Given a domain Ω divided into a mesh τ_h, for a desired order of accuracy k and with the space $\mathbb{P}_k$ of the polynomials of maximum degree k, let us define the local space $V_{k,h}^{El}$ as

$$V_{k,h}^{El} = \{v_h \in \mathrm{H}^1(El) : v_{h|\partial El} \in C^0(\partial El), \\ v_{h|e} \in \mathbb{P}_k(e)\, \forall e \subset \partial El,\ \Delta v_h \in \mathbb{P}_{k-2}(El)\}, \tag{4}$$

where h is a mesh parameter, El is an element of the mesh, ∂El is its border and e an edge. From the definition it can be seen that the base functions in the VEM space are not necessarily explicitly known for the entire domain, they are only known at the boundary of the element.

The global virtual element space is

$$\boldsymbol{\mathcal{V}}_{k,h} = \{\boldsymbol{v}_h \in \mathrm{H}_D^1(\Omega) \cap C^0(\Omega) : \boldsymbol{v}_{h|El} \\ \in \boldsymbol{\mathcal{V}}_{k,h}^{El}, \forall El \in \mathcal{T}_h\}\ . \tag{5}$$

As in FEM the discrete solutions of variational problems are searched:
Find $\boldsymbol{u_h} \in \boldsymbol{\mathcal{V}}_{k,h}$ such that

$$a_h(\boldsymbol{u}_h, \boldsymbol{v}_h) = l_h(\boldsymbol{v}_h) \qquad \forall \boldsymbol{v}_h \in \boldsymbol{\mathcal{V}}_{k,h}\ . \tag{6}$$

The discrete versions of the bilinear forms are defined element-wise

$$a_h(\boldsymbol{u}_h, \boldsymbol{v}_h) = \sum_{El \in \mathcal{T}_h} a_h^{El}(\boldsymbol{u}_h, \boldsymbol{v}_h) \tag{7}$$

$$= \sum_{El \in \mathcal{T}_h} \int_{El} \boldsymbol{\varepsilon}(\boldsymbol{u}_h) : \boldsymbol{E} : \boldsymbol{\varepsilon}(\boldsymbol{v}_h)\, dEl\ . \tag{8}$$

As the base functions in the local spaces are not explicitly known inside an element the inclusion of the projector operator is required.

Projection operator The local projector operator $\Pi_k^{El} : \boldsymbol{\mathcal{V}}_{k,h}^{El} \to [\mathcal{P}_k(El)]^2$ acting on a function $\boldsymbol{v}_h \in \boldsymbol{\mathcal{V}}_{k,h}^{El}$ is defined by

$$\underline{a}_h^{El}(\Pi_k^{El}(\boldsymbol{v}_h), \boldsymbol{p}) = \underline{a}_h^{El}(\boldsymbol{v}_h, \boldsymbol{p}) \quad \forall \boldsymbol{p} \in [\mathcal{P}_k(El)]^2\ . \tag{9}$$

In this work it is assumed that the coefficients in $\boldsymbol{E}$ are constant within each element. Although the base functions are not known in the interior of the elements, the projector can be exactly computed for functions in the local space using from the DOFs using integration by parts. The definitions of the projection operator guarantee exact results when tested against polynomials of degree up to k.

Stiffness matrix The local bilinear form needs to be decomposed into a consistency and a stability term

$$a_h^{El}(\boldsymbol{u}_h, \boldsymbol{v}_h) = \underbrace{a_h^{El}(\Pi_k^{E}(\boldsymbol{u}_h), \Pi_k^{El}(\boldsymbol{v}_h))}_{consistency} \\ + \underbrace{\mathcal{S}^{El}(\boldsymbol{u}_h - \Pi_k^{El}(\boldsymbol{u}_h)), \boldsymbol{v}_h - \Pi_k^{El}(\boldsymbol{v}_h))}_{stabilization}\ . \tag{10}$$

The consistency term approximates the bilinear form using the projection operator, while the stabilization term is applied to the high order terms ($> k$) whose contribution is left out by the projector. The later is taken simply as the scalar product of the values at the DOFs of the difference between the VEM function and its projection,

$$\mathcal{S}^{El}(\boldsymbol{u}_h - \Pi_k^{El}(\boldsymbol{u}_h), \boldsymbol{v}_h - \Pi_k^{El}(\boldsymbol{v}_h)) = \\ \tau \sum_{l=1}^{2n_{k,D}^{El}} \mathrm{dof}_{\,l}(\boldsymbol{u}_h - \Pi_k^{El}(\boldsymbol{u}_h))\, \mathrm{dof}_{\,l}(\boldsymbol{v}_h - \Pi_k^{El}(\boldsymbol{v}_h)), \tag{11}$$

where dof_l is the value at the l-th DOF, and τ is a material parameter which for linear elasticity is constant and dependent on Young's modulus and Poisson's ratio.

By defining a base for the local space $\{\boldsymbol{\varphi}_i\}_{i=1,\ldots,2n_{k,D}^{El}}$, where each function takes the value 1 at its associated DOF and 0 otherwise, the stiffness matrix results

$$\left[k^{El}\right]_{ij} = a_h^{El}(\boldsymbol{\varphi}_i, \boldsymbol{\varphi}_j) \qquad i,j = 1,...,2n_{k,D}^{El} \, . \tag{12}$$

The assembly of the global matrices system is done as in standard FEM.

Loading terms As the base functions are known on the boundaries surface load terms are treated just as in standard FEM. Volumetric terms will not be considered in this work.

3 Discontinuous Interface elements

In the framework of continuous mechanics problems which also account for explicitly considered cracks, the governing equations including the equilibrium equation, the natural and essential boundary conditions as highlighted in Eq. (1), are completed with the traction continuity on the crack surface as follows:

$$\begin{cases} \sigma \mathbf{n}_d^+ &= \mathbf{t}_c^+ \\ \sigma \mathbf{n}_d^- &= \mathbf{t}_c^- \quad \text{on}\, \Gamma_d \\ \mathbf{t}_c^+ &= -\mathbf{t}_c^- \end{cases} \tag{13}$$

where $\mathbf{t}_c$ is the cohesive traction across the crack line Γ_d, while $\mathbf{n}$ is its unit normal vector.

The above relationship is valid for any kind of discontinuous approach employed for discrete crack analysis. When zero-thickness interface elements are used for this purpose, the displacement field of the upper and lower faces of the element are given by

$$\begin{aligned} &\mathbf{u}^+ = \mathbf{V}^{int}\mathbf{U}^+ \\ &\mathbf{u}^- = \mathbf{V}^{int}\mathbf{U}^- \\ &[[\mathbf{u}]] = \mathbf{u}^+ - \mathbf{u}^- = \mathbf{V}^{int}\left(\mathbf{U}^+ - \mathbf{U}^-\right) \end{aligned} \tag{14}$$

being $\mathbf{V}^{int}$ the matrix of the interface shape functions; $\mathbf{U}^+$ and $\mathbf{U}^-$ denote the nodal displacements of the upper face and lower face, respectively, while $[[\mathbf{u}]]$ the displacement jump vector.

Using virtual work, the following equations can be derived:

$$\begin{cases} \mathbf{f}^{int,+} = \int_{\Gamma_d} \left[\mathbf{V}^{int}\right]^T \mathbf{t}_c \, d\Gamma_d, \\ \mathbf{f}^{int,-} = -\int_{\Gamma_d} \left[\mathbf{V}^{int}\right]^T \mathbf{t}_c \, d\Gamma_d. \end{cases} \tag{15}$$

The tangent stiffness matrix for a given interface element on Γ_d is given by

$$\mathbf{K}_e^{int} = \int_{\Gamma_d} \left[\mathbf{V}^{int}\right]^T \mathbf{Q}\, \mathbf{C}^t [\mathbf{Q}]^T \mathbf{V}^{int} d\Gamma_d \tag{16}$$

where $\mathbf{Q}$ is the rotation matrix needed for the transformation of the nodal displacements when the local interface coordinate system differs from the global one, and $\mathbf{C}^t$ is the tangential material modular matrix relating the stress rate vector and the rate vector of relative nodal displacement jumps, which defines the evolution of the zero-thickness interface's kinematic field.

4 Discretization of mesoscale simulations

The key feature in mesoscale simulation of heterogeneous materials is to geometrically represent the different constituents and their most relevant properties. When using normal FEM elements difficulties may appear such as the presence of small angles or edges and bad aspect ratios that lead to low-quality elements. These issues can be avoided using arbitrary polyhedral elements. Hence, an approach is proposed, where the benefits if VE's continuum elements is combined with interface elements. Main assumptions in this work are: (i) the continuum VE remain elastic throughout the entire deformation history while, (ii) the entire inelastic dissipation is localized in the two types of interfaces, mortar-to mortar and mortar-to-aggregate interfaces. For this purpose, once the specimen discretization with continuum finite/virtual elements is completed, interface elements are introduced along all matrix-to-matrix solid element joints, as well as on all matrix-to-inclusion joints.

4.1 VE's continuum elements

The strategy proposed in this work for modeling composites with embedded inclusions such as the mesoscopic structure of cementitious mixtures and concrete is presented in this section. These mesoscale structures are characterized by large aggregates embedded in mortar matrix as schematically indicated in Fig. 2.

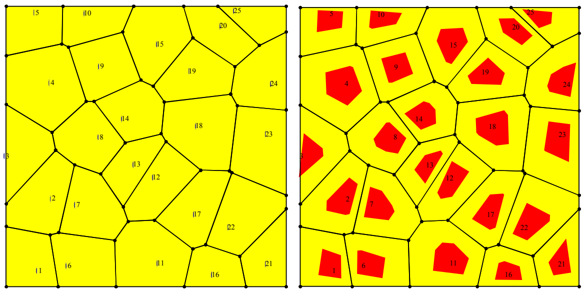
(a) (b)

Figure 2: Concrete mesoscale mesh construction.

One approach is to obtain a convex polygonal representation for representing the aggregates surrounded by the mortar matrix. These polygons can be numerically generated through the so-called Voronoi/Delaunay tessellation in a set of points, and slightly perturbed before the tessellation procedure to take into account the real aggregate distribution. Coarse aggregates are obtained by resizing and randomly rotating the Voronoi polygons. The input data for the discretization procedure mainly consist in the 2D specimen dimensions (based x height), mixture design parameters, volume fraction and parameters for controlling the shape characteristics of the aggregates to be generated.

This benefit of using of VEs, is that is capable of modeling these complex inclusions and geometries with few elements, and without the problem of element distortion.

4.2 Zero-thickness interface elements

Interface elements are added on edges of the VE mesh. Since the functions in the local VEM spaces are polynomials on the boundaries of the element, the insertion of the interface elements is the same as with standard FEM. These interfaces must form a closed path on the mesh, or else a physically inconsistent non-propagating crack would occur.

In this work, the interfaces surrounds any solid element but only in the region where the mesoscale is explicitly meshed, and therefore, a closed loop is always determined. This becomes specially useful for meshing since the process is done locally on the element. However, the effectiveness and accuracy of this procedure strongly depends on the mesh density to avoid introducing constrains to the crack evolutions during the deformation history of the concrete component. Precisely, VE are particularly convenient to be used in fine meshes composed by inclusions and characterized by highly distorted geometries as in the present case.

The material behavior used for these elements is the fracture-based rulse proposed by [12], where the traction separation law for the Cohesive zone model depend on 8 parameters: maximum normal stress, maximum tangential stress, mode I fracture energy, mode II fracture energy, two post peak softening parameters, and the ratios between final and critical opening. This model follows an intrinsic approach, which means that a high initial stiffness is provided until the critical stress is reached and then the behavior changes quickly into the softening descent.

5 Numerical analysis

A numerical example of the classical three-point bending test on a notched concrete beam is shown in this section. The geometry and boundary conditions can be seen in Figure 3. In this numerical analysis a so-called concurrent multiscale procedure is followed. Thus, the zone of the 3-point bending problem where the inelastic behavior and cracking process localize, a mesoscopic fine mesh is considered, while a macroscopic representation of the material is used for the other zones. The transition in element size was done in a smooth way in order to achieve a good flexural moment distribution, as order 1 elements were used, but VEM would have allowed for discrete changes in mesh size. Material properties in the macroscopic portion were obtained as the weighted average between those of the aggregates and the mortar. Aggregates were chosen randomly between the elements to achieve a 20% volume ratio.

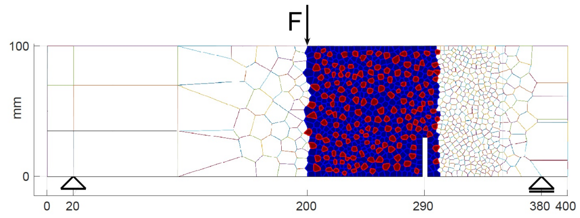

Figure 3: Three-point beam initial conditions

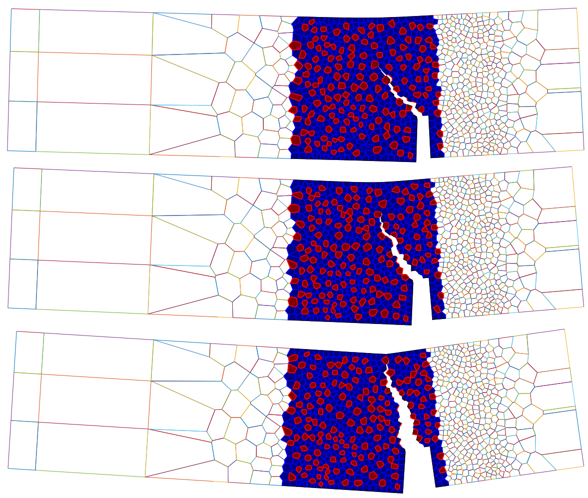

Figure 4: Crack propagation of 3 different aggregate distributions (Magnified x5)

This problem serves to assess the usefulness of the proposed. The randomness of the aggregates distribution represents adequately the randomness in concrete specimens. It affects both the initiation of the crack and the tortuosity of the cracking process. As it can be seen in Figure 3, the prediction of crack propagation and failure pattern do very much agree with experimental evidence. The method was able to reach the post-peak behavior with stable solutions and without the need of implementing more sophisticated solving algorithms. Thus, the proposed procedure for concurrent multiscale analysis of concrete failure behavior based on combining VE and IE is highly efficient and accurate for this purpose.

6 Conclusions and potential developments

Detail and accurate analyses of composite materials like concrete do require accounting for, at least, two scales of observations, the macroscopic or structural scale which defined the boundary conditions, and the mesoscopic scale which controls the failure behavior of the mixture constituents. When discontinuities and crack are involved the concurrent multiscale methods are more reliable than those based on RVE homogenizations. The flexibility of VEM meshes for modeling complex structures is very adequate to model heterogeneous mesoscopic structures like those of concrete. Thereby, aggregates do not need to be discretized but may be modeled by one single VE.

Another application of the VEM is its capability as a domain decomposition method. Due to the mesh flexibility any part of the domain can be split into several sub-domains, each one with its own new mesh, without greatly affecting the system. This particular feature makes VEM an interesting strategy to be considered in concurrent multiscale analyses of concrete failure behavior, involving macroscopic and mesoscopic scales in one single discretization, as it is proposed in this work. Moreover, the combination of VE and IE offer high efficiency to capture cracking processes in the mesoscopic zones where the inelastic dissipation localizes.

This idea can be further exploited for 'on-the-fly' re-meshing procedures. Initially a coarse mesh can be used, and refine only the critical sections as the analysis progresses. The same idea can also be applied to interface elements, adding them only around elements with high stress. Hence, the combination of VE and IE can be used for cracking analyses without modifying the formulation nor implementation, unlike complex methods like XFEM.

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