Crack analysis of mesoscale concrete by FEM using an alternative mesh overlay to represent mortar and coarse aggregate

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Abstract.
One of the main mechanisms of deterioration of concrete structures is cracking. As the shapes of the cracks are influenced by the heterogeneity of the concrete, when looking for a mechanical model that allows to determine them realistically, it is necessary to discretize the structure in mesoscale. Using the positional approach of the Finite Element Method (FEM), this work presents an alternative representation of mesoscale concrete. In this modeling, the finite element meshes that represent the coarse aggregates and the mortar are generated independently and overlapped to form the composite material. This strategy aims to make pre-processing easier, the nodes of each mesh need not be coincident and the degrees of freedom of the elements of the aggregates do not add any unknowns to the problem. To verify the efficiency of this model, it is applied to the concurrent multiscale analysis of a concrete sample, leading to responses close to the experimental ones.

Keywords: Mesoscale concrete, Embedded particles, Concurrent multiscale analysis

1 Introduction

The cracking of concrete observed in the structures is explained by the heterogeneity of the material seen at the smaller scales. The mesoscale is the scale where are observed the matrix, coarse aggregates and the interfacial transition zone (ITZ) , which is the weakest link and where degradation begins. At this scale, concrete can be understood as a composite of particles, and it is possible to relate its heterogeneity to the shape of the crack, giving it physical meaning [1]. Thus, numerical modeling at this scale leads to complex answers even with the use of simple constitutive models for each component of the material [2]. Among these behaviors are the location of cracks in less resistant regions, the effects of structure size on strength and the stochastic nature of the phenomenon.

In mesoscale modeling, strategies are divided according to the way to represent the domain, highlighting the use of discrete models and the use of continuous elements with the FEM. The Lattice Model, used by Schlangen and Van Mier [3], and the particle model, used by Bažant et al. [4], stand out in the discrete models. Using FEM, models that represent cracks using interface elements have been highlighted. For zero-thickness elements combined with cohesive models contributed López et al. [1]. Using high aspect ratio interface elements with degradation explained by a tensile damage model contributed Rodrigues et al. [5]. The results obtained in these mentioned works, as well as in several others, show that the concrete modeling in this scale leads to results close to the experimental ones. To represent the cracking of concrete, it is common to use concepts from fracture mechanics, plasticity theory or continuous damage mechanics.

In numerical simulation in mesoscale the different phases of concrete need to be discretized, so the computational effort and memory consumption are high. Therefore, analyses are limited to small samples with current computers. As cracking does not occur in the entire structure, a strategy to overcome this problem is to perform a concurrent multiscale analysis. In this case, the structure is divided into subdomains where each one is discretized in a scale and only the most critical places are modeled in the smallest. Lloberas-Valls et al. [6] highlight that the entire structure is processed simultaneously and the global equilibrium and displacement compatibility are valid for the entire domain, resulting in a strong coupling between the scales. The representation of concrete cracking through concurrent multiscale analysis was used by Unger and Eckardt [2], Lloberas-Valls et al. [6], Rodrigues et al. [7] and Rodrigues et al. [8], among other works, presenting good quality responses and reduction of the computational cost. The main challenges are identifying the regions to be represented at each scale and correctly linking these subdomains. Furthermore, although the computational cost has reduced compared to mesoscale modeling, it remains high. Looking for more reduction in processing time, Rodrigues et al. [7] and Rodrigues et al. [8] present a mesh adaptation strategy to represent the mesoscale only where and when the stress becomes critical.

In addition to the limitation caused by the computational cost, cracked concrete can present displacements or rotations that make the equilibrium of the current configuration of the body not approximately equal to the initial configuration. This behavior was observed in reinforced concrete frame corners by Rabczuk and Belytschko [9]. Under these conditions, the simulation must be geometrically exact in order to obtain results that are closer to the correct ones.

In this work, a computational code is developed for the analysis by FEM of the phenomenon of crack initiation and propagation in concrete structures using the concurrent multiscale analysis technique. An alternative form is used to model the mesoscale in which the meshes representing the mortar and coarse aggregate are generated independently and superimposed to form the composite. The goal is to facilitate the pre-processing step. Furthermore, the finite elements that represent the aggregates do not add degrees of freedom to the problem, therefore they also contribute to the reduction of computational cost of the analysis. The constitutive model that represents degradation comes from the continuum damage mechanics. It is applied to interface elements positioned between the mortar elements that serve as possible paths to the cracks and allow them to be represented in a discrete way. To improve the quality of the answers, the formulation used in the implementation is geometrically exact. It is a positional approach to FEM developed by Coda and Greco [10]. The code developed is used in a multiscale concurrent analysis of a $2D$ concrete sample. The obtained response is compared with the numerical result obtained with the same code representing all the mesoscale components explicitly in the same mesh and studies available in the literature.

2 Numerical Modeling

2.1 Meshes for macroscale and mesoscale

In the concurrent multiscale strategy adopted, it is necessary to create for the macroscale a mesh for the concrete material and for the mesoscale meshes to represent the mortar, the coarse aggregates and the interface elements that can be crack paths. As in the macroscale there is only one type of material, only a regular mesh with adequate mechanical properties is created. For the mesoscale, before generating the mesh, closed geometries with positions, dimensions and random shapes are inserted to represent the coarse aggregates. Then regular meshes are created for the matrix and the particles. Finally, between the elements of the matrix, interface elements are inserted. When the particles are in the same mesh as the matrix, the interface elements between these phases represent the ITZ. It is noteworthy that ITZ is neglected from the analysis when the phases are in different meshes that are superimposed.

To define the aggregates, they are randomly generated using the strategy presented in Wriggers and Moftah [11] and used in Rodrigues et al. [5]. The developed code can generate aggregates in the form of regular polygons with different numbers of sides. To define the dimension of each aggregate, the Fuller and Thompson [12] curve is used.

To create the interface elements, the mesh fragmentation technique presented in Manzoli et al. [13] is used, which is divided into 3 main steps. Step 1 consists of generating the regular mesh for the entire sample. Step 2 consists of reducing the dimensions of all elements leaving an empty space between them for the positioning of the interface elements. Finally, in Step 3 the interface elements are inserted into these spaces. Manzoli et al. [13] showed that when the smallest height of these elements approaches zero, they are suitable for representing discontinuities. This happens because, in the limit, the behavior observed is the same as the continuum strong discontinuity approach, presented in Oliver et al. [14]. Therefore, they can be applied in the analysis of concrete cracking. They just need to have a high aspect ratio, small height and an inelastic behavior, which in this work is represented by a damage model.

2.2 The Finite Element Method based on positions

The positional approach is a naturally non-linear geometric version of FEM in which the unknowns are the element node coordinates rather than the displacements used in the classical method. It emerged in the works of Bonet et al. [15], who used positions such as unknowns, and Coda and Greco [10], which they proposed the method and applied to $2D$ frame elements.

The method is deduced based on the principle of stationarity of mechanical energy, considering the variation of positions. This principle establishes that in the equilibrium of the body, the first variation of mechanical energy is null. This work is restricted to static problems, so that mechanical energy is composed of the potential energy of external forces and deformation energy. The first positional variation of these parcels represents the external and internal force vectors respectively. The internal force vector is not obtained from a linear relationship between the stiffness matrix and the nodal positions, so the Newton-Raphson method is used for the iterative solution of the problem. In it, it is necessary to previously know the initial and current position of the body, where the latter is known by trial. To use the technique, it is necessary to calculate the internal force vector and the tangent stiffness matrix for each trial. These terms are obtained as a function of the specific deformation energy, and depend on the constitutive model and the type of element used.

The elements used in this work are $2D$ solids with linear approximation. The way to calculate the internal force vector and the tangent stiffness matrix of these elements is detailed in Coda [16]. The constitutive model used is that of Saint-Venant-Kirchhoff (SVK), whose specific deformation energy is given by

$$\Psi(E) = \frac{1}{2} E_{kl} \mathfrak{C}_{klij} E_{ij}, \tag{1}$$

where E is the Green deformation and $\mathfrak{C}$ is the elastic constitutive tensor. This model is suitable for describing the behavior of materials that have large displacements and moderate strains.

2.3 Coupling matrix and particles

The strategy used allows the representation of reinforcements with perfect adherence without adding degrees of freedom to the problem and without the need for coincidence of nodes of the elements of the matrix and particles discretization. The idea of the strategy appears Vanalli et al. [17] to couple simple bar and matrix elements using the traditional FEM and considering perfect adhesion. Sampaio et al. [18] extended the idea to the positional formulation of the FEM and used it for simple bar elements with any order of polynomial approximation. Using the same strategy, Paccola and Coda [19] were successful in coupling particles and matrix to model composites with elastic behavior. The formulation used here is the one presented in Paccola and Coda [19] to connect the matrix and particles with perfect adhesion.

The technique consists of representing the nodal positions of the elements of the particles using the shape functions of the elements of the matrix. For this, it is necessary to determine the dimensionless coordinates of the node elements of the particles within the matrix elements that they are superimposed on in the initial configuration. Once these coordinates are determined, all the nodal information of the elements of the particles is written as a function of the coordinates of the nodes of the matrix. The deductions presented in Paccola and Coda [19] allow us to conclude that the internal force and the tangent stiffness matrix of the particles can be calculated as a function of their own nodes and then distributed over the nodes of the elements of the matrix. For this, they are weighted by the shape functions applied to the dimensionless coordinate point corresponding to each node of the elements of the particles within the elements of the matrix. Thus, the global internal force vector and the tangent stiffness matrix are obtained by adding the values obtained for the elements of the matrix with those of the particles thus distributed.

2.4 Damage model

The degradation is explained by a tensile damage model applied to the interface elements used by Manzoli et al. [13]. The bulk elements show linear elastic behavior. As in this model only the tension component of the stress tensor is used, it is limited to cases where the mode I fracture predominates. The criteria for the existence of damage ϕ is given by

$$\phi = \sigma_{nn} - q(r) \leq 0, \tag{2}$$

where σ_{nn} is the Cauchy stress normal to the major base of the interface element, q and r are the stress and strain-like internal variables, respectively. The function $q(r)$ defines the softening law. Dividing all terms of ϕ by $(1-d)$, the damage criterion for the effective stress is given by

$$\overline{\phi} = \overline{\sigma}_{nn} - r \leq 0, \tag{3}$$

where was made $(r = q/(1-d))$ to control the elastic domain in the space of effective deformations. Isolating d, the damage variable is given by

$$d = 1 - \frac{q(r)}{r}. \tag{4}$$

In the damage evolution, in the loading–unloading conditions, one must respect the relations given by

$$\overline{\phi} \leq 0, \dot{r} \geq 0 \text{ and } \dot{r}\overline{\phi} = 0, \tag{5}$$

where $\dot{r}$ is the rate of change of r along time. To ensure consistency condition,

$$\dot{r}\dot{\overline{\phi}} = 0 \text{ if } \overline{\phi} = 0. \tag{6}$$

Under these conditions, for a pseudo-time t associated with the loading process, the variable r is always given by the highest value between $\overline{\sigma}_{nn}$ up to that moment and the initial value of the process r_0 given by the tensile strength f_t of the material. So it can be written as

$$r = max(\overline{\sigma}_{nn}(s), r_0) \ | \ s \in [0, t]. \tag{7}$$

To represent the softening, the same exponential law already used successfully by Rodrigues et al. [5] for mesoscale concrete was chosen. It is given by

$$q(r) = f_t \exp\left(\frac{f_t^2}{G_f \mathbb{E}} h(1 - r/f_t)\right), \tag{8}$$

where h is the smallest height of the interface element, G_f is the fracture energy for mode I, and $\mathbb{E}$ is the Young's modulus of the material.

The damage implementation algorithm is adapted from the version used by Manzoli et al. [13] and it is the implicit-explicit integration scheme (IMPL-EX) developed in Oliver et al. [20]. As in the implemented constitutive model the second Piola-Kirchhoff stress tensor is used, it is necessary to calculate the Cauchy stress tensor through it. It is given by

$$\sigma = \frac{1}{J} A \cdot S \cdot A^t, \tag{9}$$

where A is the gradient of the change of configuration function and J its determinant.

3 Numerical example

3.1 Three-point bending test - multiscale modeling

In this example, a three-point bending test is simulated on a simple concrete beam with a notch in the middle of its length. This beam was experimentally tested by Kormeling and Reinhard [21]. The geometry and boundary conditions of the structure are shown in Fig. 1. The beam thickness is 100 mm. The load is applied in the form of prescribed displacement δ at the midpoint of the upper edge of the beam, where the reaction force F is observed. For this type of structure, the maximum tensions occur in the middle of the span, so the crack should start at the notch and develop approximately vertically up to the upper edge. Therefore, the mesoscale was represented only in a central region with a length equal to 50 mm and height equal to the beam. Information about the coarse aggregate were unknown and were taken arbitrarily. They are represented by regular polygons of 5, 6, 7 and 8 sides and diameters ranging from 4 mm to 8 mm.

Two models with different representations of the mesoscale named Same Mesh Model (SM Model) and Overlapping Mesh Model (OM Model) were analyzed. In the SM Model, mortar and coarse aggregate are represented in the same mesh and the interface elements at the edges of the particle have ITZ properties. In the OM Model, a mesh is created to represent the matrix and another to represent the coarse aggregates overlaying it. The coarse aggregates do not add degrees of freedom and the adhesion to the matrix is perfect. In both cases, the macroscale mesh and the distribution of aggregates were the same. The coupling between the meshes of the scales in both cases was done directly by gradually reducing the size of the macroscale elements until reaching the dimension of the mesoscale elements. For the SM Model the analysis has 7003 nodes and 10188 elements. For the OM Model the analysis has 8735 nodes and 11726 elements, where 749 nodes are in the particles and do not add degrees of freedom to the problem.

The macroscale concrete presents Young's modulus $E = 20000$ MPa and Poisson's ratio $\upsilon = 0.20$, values obtained experimentally by Kormeling and Reinhard [21]. The aggregate was adopted with $E = 37000$ MPa $\upsilon = 0.18$, which are identical properties to those used by Unger and Eckardt [2] for represent a mesoscale concrete of the same Young's modulus. Knowing E and υ of concrete and aggregate, these values were used to obtain these properties for the mortar using the parallel model of Counto [22], resulting in $E = 15172$ MPa and $\upsilon = 0.21$. For the interface elements, the same E of the mortar and $\upsilon = 0.0$ are used, in addition it is also necessary to calculate G_f and f_t to be used in the damage model. For concrete, Kormeling and Reinhard [21] determined that $G_f = 0.113$ N/mm and $f_t = 2.4$ MPa. For the SM Model, G_f and f_t were estimated for interfaces representing mortar and representing ITZ. It was assumed that the average of the values of each parameter, considering their values for ITZ and mortar, results in the measured value for concrete, following Rodrigues et al. [5]. Thus, starting from the known values for concrete, for the interfaces representing mortar, was adopted $G_f = 0.161$ N/mm and $f_t = 3.429$ MPa and for those representing ITZ, was adopted $G_f = 0.081$ N/mm and $f_t = 1.714$MPa. For the OM Model, as there is only one type of interface element, G_f and f_t must have an intermediate behavior between ITZ and mortar, we chose to use $f_t = 2.4$ MPa e $G_f = 0.113$ N/mm, which are the values experimentally determined for concrete. The analyzes were carried out considering plane stress state with displacement control. The prescribed displacement has been divided into 400 increments.

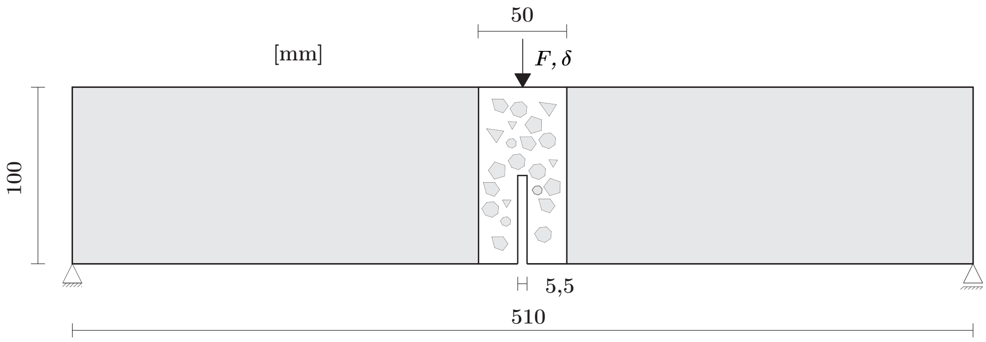

Figure 1. Geometry and boundary conditions

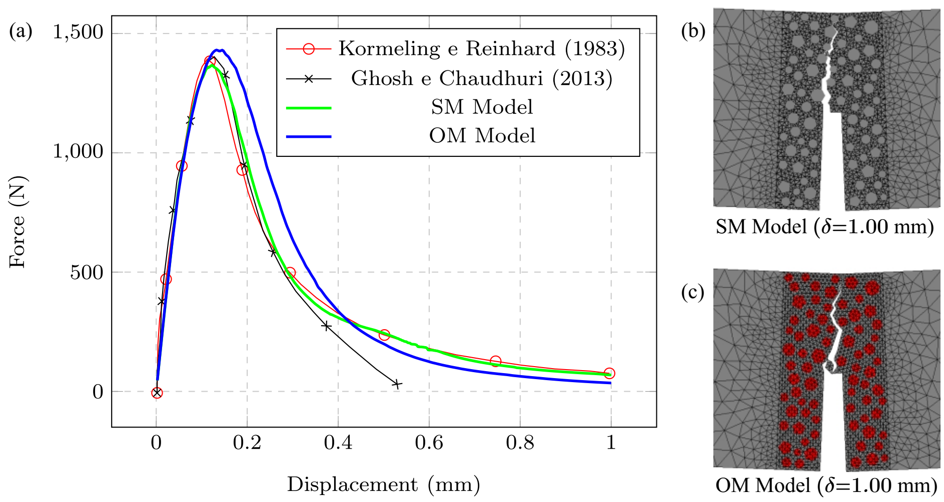

Figure 2. Results obtained for the three-point bending test: force-displacement curves (a) and cracks at the end of the analysis for SM Model (b) and OM Model (c)

In Fig. 2 (a) the graphs relating the reaction force F with the applied displacement δ obtained for the models considered are presented. In general, it was possible to observe a good agreement between the results obtained in this work and the experimental results of Kormeling and Reinhard [21] and the numerical results of Ghosh and Chaudhuri [23]. The curve obtained with the SM Model fit the experimental results well. It was even able to follow it until the end of the analysis, which is attributed to the exponential nature of the softening curve adopted in the damage model. For the OM Model the curve was also close to the experimental one, however, it presented a higher peak value and a softening curve with a slower drop. This difference is attributed to the fact that in this model there are more simplifications than in the SM Model. Among them, the representation of the mesoscale with superimposed particles, the use of tensile strength and fracture energy of concrete in the damage model and the absence of the ITZ representation. In Fig. 2 (b) and (c) are presented the cracks at the end of the analysis for the SM Model and OM Model respectively. In both cases the crack developed vertically between the aggregates as expected. In the OM Model, cracks do not pass on the face of the aggregate as it occurs experimentally and can be observed in the SM Model. This is due to the lack of coincidence of the matrix and aggregate meshes and the non-representation of ITZ. The limitations presented in the OM Model are greater than those of the SM Model for both the response curve and the crack shape. But the influence on the result is low and as this strategy brings advantages in the sense of easier mesh generation and reduction of the problem degrees of freedom, it is an alternative for mesoscale modeling of concrete or other composites of particles with quasi-brittle behavior.

4 Conclusions

In this work, an alternative for mesoscale concrete modeling was presented in which the coarse aggregates do not add degrees of freedom to the problem. The technique was applied to a beam under bending leading to good results, both in relation to the response curve of the structure and the shape of the discrete crack that develops. Therefore, the capability of the code developed and the modeling strategy used to represent the cracking of simple concrete in concurrent multiscale for structures in which the Mode I of fracture predominates were confirmed. Regarding the positional FEM and the SVK constitutive model, as the results were good, it is concluded that the code can be applied to the simulation of cracking of structures in which geometric nonlinearity is important.

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