23rd ABCM International Congress of Mechanical Engineering
December 6-11, 2015, Rio de Janeiro, RJ, Brazil

NUCLEATION AND CRACK PROPAGATION BY GENERALIZED FINITE ELEMENT METHOD BASED ON A COMBINATION OF CONSTITUTIVE AND KINEMATIC APPROACHES

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Abstract. *This paper presents computational simulations of problems concerning damage and fracture mechanics in quasi-brittle materials. The physically nonlinear analysis is started using the standard Finite Element Method, where the nucleation phenomenon is assessed through constitutive methods based on elastic degradation, while crack propagation is evaluated through kinematic method that incorporates the discontinuities. Such discontinuities are represented using enriched interpolations based on Generalized Finite Element Method (GFEM). This combination of constitutive and kinematic methods has the advantage of not having to pre-set crack path or reset the mesh during analysis. The relationship between stresses and displacements in the crack path is based on the concept of cohesive or fictitious crack, in particular the Hillerborg model, in which all the inelastic deformation (occurring in the fracture process zone) are represented on a line through the cohesive forces acting on the crack, or in a fictitious crack extension. The numerical simulations are performed using an interactive graphical software that integrates mesh generator, constitutive models, nonlinear equation solvers and post-processor. Such a software results from the expansion of the project INSANE (INteractive Structural ANalysis Environment), an open source computational platform developed by the Structural Engineering Department of Federal University of Minas Gerais.*

Keywords: *Damage and Fracture Mechanics, Quasi-Brittle Materials, Physically Nonlinear Analysis, Constitutive Method, Generalized Finite Element Method.*

1. INTRODUCTION

This paper presents a proposal for modeling the crack nucleation and propagation in quasi-brittle materials. Based on the concepts of damage and fracture mechanics, the analysis can be processed in three stages, namely: medium degradation, nucleation of cracks and crack propagation.

The degradation phenomenon can be analyzed by constitutive methods. These methods consider that the medium, even though degraded, remains continuous, but that the properties of the material are modified in the regions where the efforts are upper than given strength parameters. This approach allows, as an initial step, modeling the medium deterioration, without considering the existence of previous cracks. The next steps of the analysis, however, may result in a degradation level that justifies, in order to make a more realistic simulation, the introduction of discontinuities into the geometry (formation of discrete cracks), rather than, as initially, only a distributed degradation. This threshold stage is said nucleation of cracks and should be evaluated from the definition of a measure that take into account the variables of the constitutive model. It is also desirable that such measure be common to any constitutive method, i.e. that the measure be independent of a particular constitutive method.

The discontinuities may be considered during the analysis by numerical methods based on geometrical representation, which require the prior definition of the crack path or resetting the mesh. On the other hand, the discontinuities may also be considered by numerical methods based on non-geometric representation in which the effects of the presence of cracks in the fields of displacement, strain and stress are embedded into the element, requiring its reformulation.

This reformulation can be performed by means of the Generalized Finite Element Method, a method that allows the enrichment of the partition of unit functions so that the discontinuities become incorporated into the approximate solution.

The enrichment process can incorporate a discrete constitutive model (relation between stress and displacement on the crack path). Such model is based on the concept of cohesive (or fictitious) crack, in particular Hillerborg model, in which all the inelastic deformation (which occur in the fracture process zone) are represented in a line through the cohesive forces acting in the crack, or in a fictitious extension of the crack.

An analysis with the above characteristics is said to be physically nonlinear analysis and demands appropriate computing resources. The INSANE (*INteractive Structural ANalysis Environment*) computational system is a free software project, implemented in Java language according to the Object-Oriented Programming paradigm, developed at the Structural Engineering Department of the Federal University of Minas Gerais (UFMG) and available at `http://www.insane.dees.ufmg.br`. This work is inserted in the expansion project of such system, which has several resources for physically nonlinear analysis and could be improved to permit the analysis proposed here, because it consists of a segmented computational environment, friendly to changes and scalable in complexity.

2. NUMERICAL MODELS FOR CRACKING

Ingraffea and Wawrzynek (2004) present a very interesting classification of the main numerical methods used in various applications of Fracture Mechanics over the last decades, Fig. 1. In this classification, the authors are concerned in dividing those numerical methods in two main groups, which are distinguished by the way they represent the crack propagation. In the first group, the crack is a geometric entity represented by the numerical model. As a consequence of the crack propagation the geometry of the model and the finite element mesh may change. In the second group, the crack is indirectly represented, and neither the geometry nor the mesh of the model need to be changed with the crack propagation. This so-called Non-Geometrical Representation, scope of this paper, embraces two different approaches. In the approach based on the constitutive methods the stiffness of the material is degraded in the damaged region to simulate the discontinuity of the displacement field caused by cracking. In the Kinematic Methods, the effect of cracking over the displacement and strain fields is embedded into the elements, locally in the element shape functions, or globally in the element nodes.

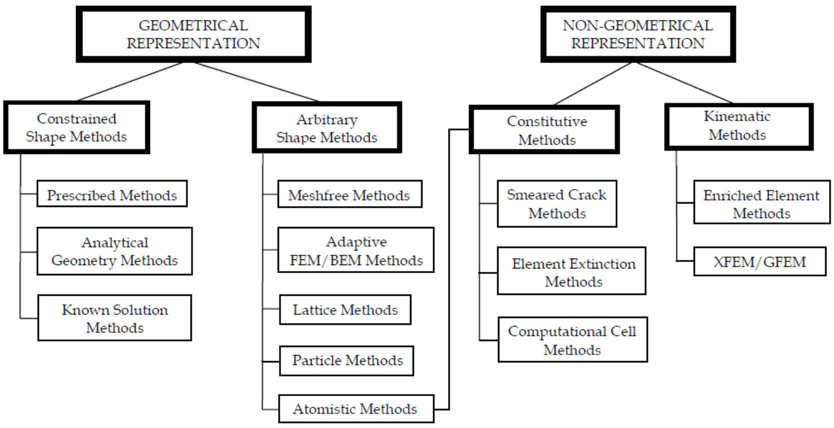


Figure 1. A taxonomy of methods for modeling of cracking (Ingraffea and Wawrzynek, 2004)

3. CONSTITUTIVE METHODS

There are several models proposed, considering smeared deterioration in quasi-brittle materials, among them stand out the Smeared Cracking and Damage Models. In these models, the material is idealized as a continuous medium with degradation due to the cracking process.

Generally, Smeared Cracking Models consider that the cracked region is formed by a set of small cracks parallel to each other. Thus, a cracked region would be represented by a set of finite elements with orthotropic behavior. That is, by positioning the local system of the constitutive tensor of these elements in perpendicular and parallel directions to the crack plane, different values can be adopted for the elastic modulus in these directions, therefore characterizing an orthotropic finite element (Pitangueira, 1998). Then, using an orthotropic constitutive tensor, the stiffness of the elements in the cracked area presents a gradual deterioration, and the cracking effect of it is numerically reproduced with no need of changes in the mesh (Wolff, 2010). The gradual deterioration is monitored by relations between stresses and displacements and material strength limits and fracture mechanics parameters are used in the formulation (Pitangueira, 1998).

The smeared cracking models can be classified into two categories, according to Rots (1988): fixed or rotating cracking direction models. The model with fixed direction considers that, once started, the crack has fixed guidance throughout the process of propagation. The model with rotating direction admits that the cracks can rotate according to the orientation of the principal strain/stress.

The damage models, according to Murakami (2012), in the case of random distribution of microvoids or isotropic distribution of spherical voids, the damage state is considered to be isotropic and can be represented by a damage scalar variable. On the other hand, when the microvoids have a oriented geometry or configuration, the damage state is anisotropic and damage scalar variable cannot be applied accurately, employing tensor damage variables, unless the void density is small (Lemaitre, 1992).

Carol *et al.* (1994) presents a unified elastic degradation and damage theory based on loading surface, whose formulation is based on hypothesis of a single loading function. Using this theory, the most important scalar damage models found in the literature of that time were reinterpreted and reformulates.

According to Penna (2011), damage can be defined as the appearance, or "nucleation", and advance process of microvoids and microcracks until material failure. That is, a given intact material, when submitted to strains, evolves into a state of microcracks until macroscopic failure. At microscale, damage is seen as a discontinuity of the material, and at larger scales, the material can be treated as continuous.

The continuum damage mechanics, in accordance to Lemaitre (1992), studies the macroscopic behavior of a material, considering it as homogeneous. The consideration of a continuous medium is made by defining a "Volumetric Representative Element" (VRE), whose magnitude is such that the degraded material medium can be treated as homogeneous.

Physically, the damage can be seen as plastic or permanent deformations, caused by the deterioration of the physical properties of the material (Penna, 2011).

According to Penna (2011) the empirical study of the damage in different materials led to the development of various constitutive models that are able to describe their behavior.

It is observed that the degradation is not a directly measurable physical quantity, however, it can be determined by gradually reducing a mechanical property such as, for example, elastic modulus, and the degraded medium can be considered isotropic, orthotropic, or even anisotropic.

A theoretical and computational framework for constitutive models based on elastic degradation was developed by Penna (2011) into the INSANE system. Several classical models to deal with the material degradation were discussed in the context of this framework and were implemented in INSANE. Among them, some damage models and a plasticity model. Smeared cracking models were reformulated, considering multiple loading functions and a general degradation rule, adapting them to the framework. It includes: Elastoplastic Model with von Mises Yield Criterion; Mazars Isotropic Damage Model (Mazars, 1984); Mazars and Lemaitre Isotropic Damage Model (Mazars and Lemaitre, 1984); Simo and Ju Isotropic Damage Model (Simo and Ju, 1987); Ju Isotropic Damage Model (Ju, 1989); Lemaitre and Chaboche Isotropic Damage Model (Lemaitre and Chaboche, 1990); de Vree Isotropic Damage Model (de Vree *et al.*, 1995); Smeared Cracking Models, with Fixed or Rotating Direction; Smeared Damage Model by de Borst and Gutierrez (de Borst and Gutierrez, 1999); Volumetric Damage Model (Penna, 2011).

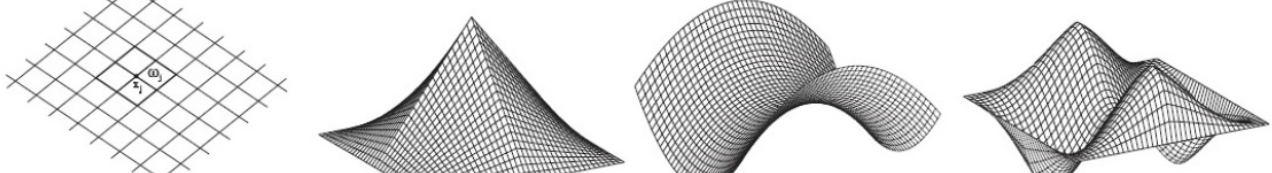
4. GENERALIZED FINITE ELEMENT METHOD - A KINEMATIC METHOD

The Generalized Finite Element Method (GFEM) (Strouboulis *et al.*, 2000) is a numerical method of non-geometrical kinematic representation, according to the classification proposed by Ingraffea and Wawrzynek (2004) (Fig. 1). It is adopted here for analysis of crack propagation, allowing that the effects of discontinuities in the fields of displacements and strains be embedded in the enriched interpolation functions.

The GFEM can be understood as a variation of the conventional Finite Element Method (FEM). The strategy used in GFEM is to employ Partition of Unity (PU) functions that, enriched, define the shape functions. The choice of the PU functions depends on the type of problem to be analyzed (Barros, 2002; Alves, 2012).

The use of conventional FEM functions (e g., the Lagrangian functions) as PU functions, besides facilitating the application of the method, ensures stability to the analysis, directly checking the boundary conditions (Alves, 2012).

To better understand the method, let be considered a conventional finite element mesh defined from a set of n nodal points $\{\mathbf{x}_j\}_{j=1}^{n}$, as can be seen in Fig. 2(a), for the case of a two-dimensional domain. It is defined then the region or cloud ϖ_j, formed by all the elements that share nodal point $\mathbf{x}_j$.



(a) Cloud $\omega_j = \{\mathcal{K}_e | \bar{\mathcal{K}}_e \supset \boldsymbol{x}_j\}$ (b) Partition of Unity Function $\mathcal{N}_j(\boldsymbol{x})$ (c) Local Function $L_{ji}(\boldsymbol{x})$ (d) $\phi_{ji}(\boldsymbol{x}) = \mathcal{N}_j(\boldsymbol{x}) \times L_{ji}(\boldsymbol{x})$

Figure 2. Enrichment strategy of the cloud ϖ_j (Barros, 2002)

The set of Lagrange interpolation functions associated with the node $\mathbf{x}_j$, obtained through the Finite Element Method, defines the function $N_j(\mathbf{x})$, whose support corresponds to region ϖ_j, Fig. 2(b).

A set of enrichment functions, which are called *local functions* (Alves, 2012) and can be specific to a particular type of problem (Fig. 2(c)), consists of q_j linearly independent functions defined for each node $\mathbf{x}_j$ with support on the cloud ϖ_j, as in Eq. (1).

$$I_j \overset{def}{=} \{L_{j1}(\mathbf{x}), L_{j2}(\mathbf{x}), ..., L_{jq}(\mathbf{x})\} = \{L_{ji}(\mathbf{x})\}_{i=1}^{q} \tag{1}$$

with $L_{j1}(\mathbf{x}) = 1$

At the end of the process, the shape functions $\phi_{ji}(\mathbf{x})$ from GFEM, shown in Fig. 2(d), are associated with the node $\mathbf{x}_j$, and are built by enriching the PU functions corresponding to the cloud ϖ_j, as shown in Fig. 2(a), by the components of the set I_j, from Eq. (1). So, $\phi_{ji}(\mathbf{x})$ can be easily obtained by the product of the basic functions that form the PU (Fig. 2(b)), which are obtained through the conventional FEM, by the enrichment functions, represented in Fig. 2(c), according to Eq. (2).

$$\{\phi_{ji}\}_{i=1}^{q} = N_j(\mathbf{x}) \times \{L_{ji}(\mathbf{x})\}_{i=1}^{q} \tag{2}$$

with no summation in j.

The functions of the set Eq. (1) can be polynomial or not, being selected as the type of problem that is being analyzed (Alves, 2012). A generic approximation $\tilde{\mathbf{u}}(\mathbf{x})$ is obtained by the following linear combination of the shape functions (Eq. (3)):

$$\tilde{\mathbf{u}}(\mathbf{x}) = \sum_{j=1}^{N} N_j(\mathbf{x}) \left\{ \mathbf{u}_j + \sum_{i=2}^{q} L_{ji}(\mathbf{x}) \mathbf{b}_{ji} \right\} \tag{3}$$

where $\mathbf{u}_j$ and $\mathbf{b}_{ji}$ are nodal parameters associated with each component $N_j(\mathbf{x})$ and $N_j(\mathbf{x}) \cdot L_{ji}(\mathbf{x})$, respectively.

As a final result of the process, it is obtained the product function, which presents the approximating characteristics of the local approximation function, while inheriting the PU compact support (Alves, 2012).

The utilization of this method provides employment of FEM functions for the PU as well as improves the analysis of problems in which the enrichment with special functions (with step function, for example) presents significant advantage (Barros, 2002).

As a classical step function stands out the Heaviside function. Different definitions have been adopted for the Heaviside function over the years (Mohammadi, 2008). The first type of Heaviside function $H(\xi)$ can be defined as:

$$H(\xi) = \begin{cases} 1, & \forall\, \xi > 0 \\ 0, & \forall\, \xi < 0 \end{cases} \tag{4}$$

Thus, adopting the Heaviside function as enrichment function of the Generalized Finite Element Method it is possible to describe the displacement field decomposed into two parts, one continuous and one discontinuous (Wolff, 2010), allowing simulate the presence of discontinuities in the mesh. According to Mohammadi (2008), Eq. (3) can be writing as,

$$\tilde{\mathbf{u}}(x) = \sum_{j=1}^{N} N_j(\mathbf{x}) \mathbf{u}_j + \sum_{k=1}^{m} N_k(\mathbf{x}) H(\xi) \mathbf{b}_k \tag{5}$$

where $\mathbf{u}_j$ is the regular degrees of freedom in the finite element method, $\mathbf{b}_k$ is the added degrees of freedom and $H(\xi)$ is the discontinuous enrichment function.

According to Wolff (2010), indeed, regular degrees of freedom $\mathbf{u}_j$ represent the continuous part, while the additional degrees of freedom $\mathbf{b}_k$ represent the jump displacement along the discontinuity.

5. DISCRETE CONSTITUTIVE MODEL

The discretized constitutive model (relationship between the stress and the displacement in the crack path) is based on the concept of cohesive (or fictitious) crack. In Hillerborg model (Hillerborg *et al.*, 1976), all the inelastic deformation (which occur in the fracture process zone) are represented in a line through the cohesive forces acting in the crack, or in a fictional extension of the crack (Fig. 3).

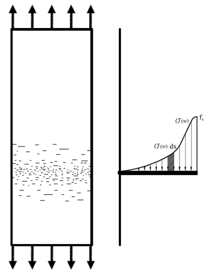


Figure 3. Strain localization in a line of cracking (Adapted from Wolff (2010))

The constitutive model is defined by a system of local orthogonal coordinates, in which the vectors n and s represent directions normal and parallel to the crack, respectively (Fig. 4).

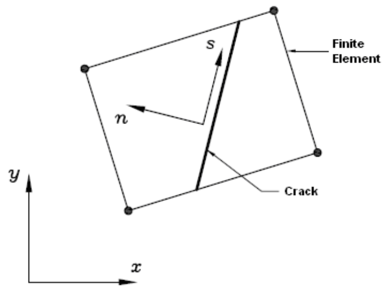


Figure 4. Local coordinates system of discontinuity within a finite element (Wolff, 2010)

It is intended that the degradation of the material surrounding the crack remains evaluated by constitutive methods, even with the introduction of the crack.

6. PRELIMINARY RESULTS

At the present stage of research, a structure can be analyzed in the INSANE system, by evaluating the process of degradation of the material in a distributed manner, adopting constitutive methods, according to section 3.

It is also allowed the introduction of discontinuities in the displacement field by Generalized Finite Element Method, as section 4.

However, such discontinuities are still input data of the analysis. The next step will be to introduce the discontinuity from the identification of the threshold stage of nucleation of cracks by defining a measure of nucleation, as well as the propagation of the cracks and consideration of cohesive law governing its opening.

To illustrate the current state of research, it is reproduced an example presented in Penna (2011), as shown in Fig. 5.

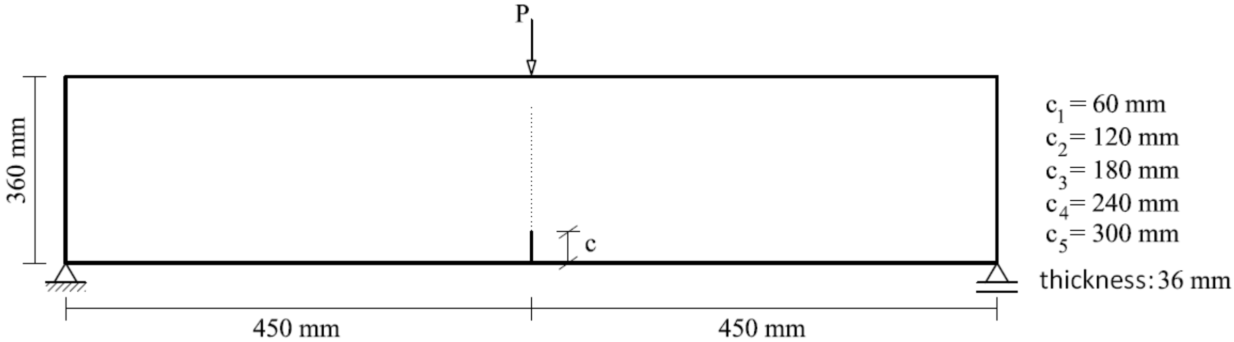


Figure 5. Geometric configuration (Penna, 2011)

This example evaluates the structural ductility of a beam subjected to three point bending. From an initial crack growth, the effect of changing the effective height of the beam in its structural behavior is evaluated. The beam dimensions are kept constant and the crack length is increased in each analysis (Penna, 2011).

In Penna (2011) was made use of nodal duplication, however, here the discontinuity will be through the Heaviside function by Generalized Finite Element Method (section 4).

The fixed smeared cracking model with Carreira and Chu (1985) law, for compression, and Boone *et al.* (1986) law, for tension, was used in the modeling. The following parameters were used: $E_0 = 44000.0N/mm^2$; $\upsilon = 0.2$; $f_c = 40.0N/mm^2$; $f_t = 3.8N/mm^2$; $\epsilon_c = 0.0018$; $G_f = 0.164N/mm$; $h = 100.0mm$ and $\beta_r = 0.05$.

The nonlinear analysis was performed using cylindrical arc length control method with initial load factor of 500.0, reference load $P = 1.0N$ and tolerance 1×10^{-4}.

The finite element mesh (Fig. 6(a)), built with four nodes quadrilateral elements of size $60 \times 60mm$, is kept constant, except for the initial crack, which is inserted into the mesh by setting its start and end points. It was implemented in INSANE system, algorithm responsible for determining the nodes that must be enriched for simulation of discontinuity.

The user interface for the introduction of discontinuities, as well as the mesh with the representation of a discontinuity, are illustrated in Fig. 6(b).

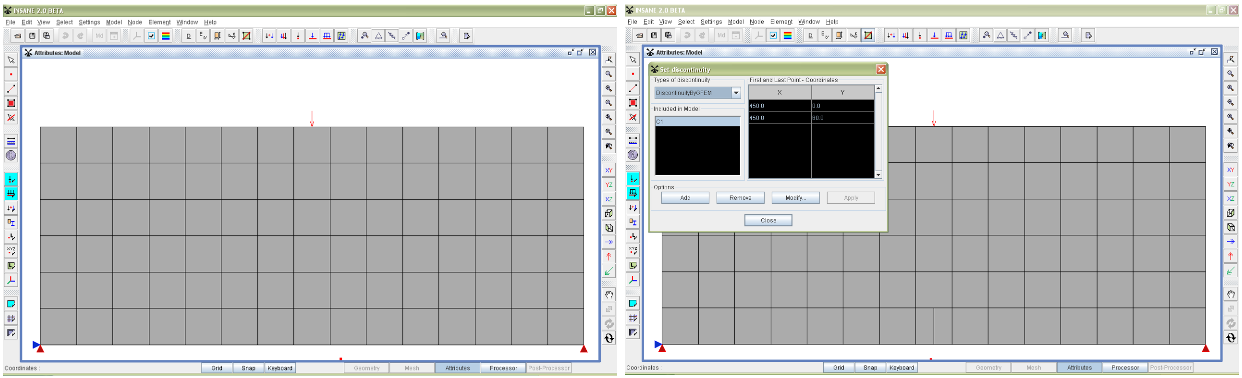


Figure 6. (a) Finite element mesh (plane stress) (b) Creation and representation of a discontinuity

The equilibrium paths for the horizontal displacement of the right support are shown in Fig. 7. Each path refers to a crack size ($c_0 = 0mm$, $c_1 = 60mm$, $c_2 = 120mm$, $c_3 = 180mm$, $c_4 = 240mm$ and $c_5 = 300mm$).

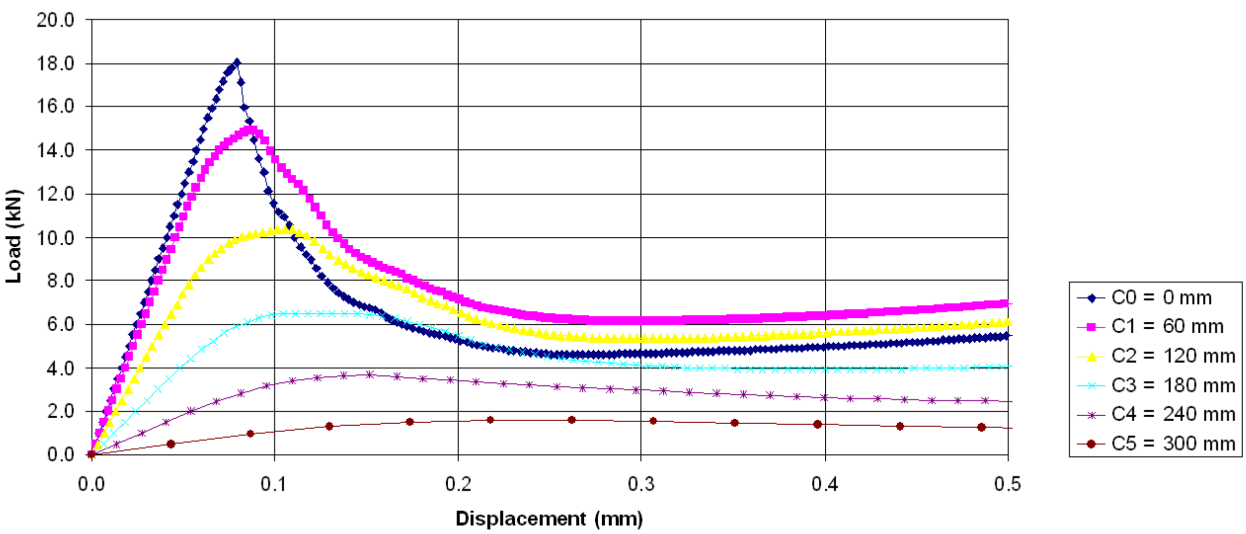


Figure 7. Equilibrium paths

As can be seen in Fig. 7, the effect of changing the effective height of the beam in its structural behavior can be understood. The mesh deformed shape for the steps 25 ($1.05kN$), 50 ($1.41kN$), 75 ($1.15kN$) and 100 ($1.16kN$) in case of discontinuity C5 are presented in Fig. 8.

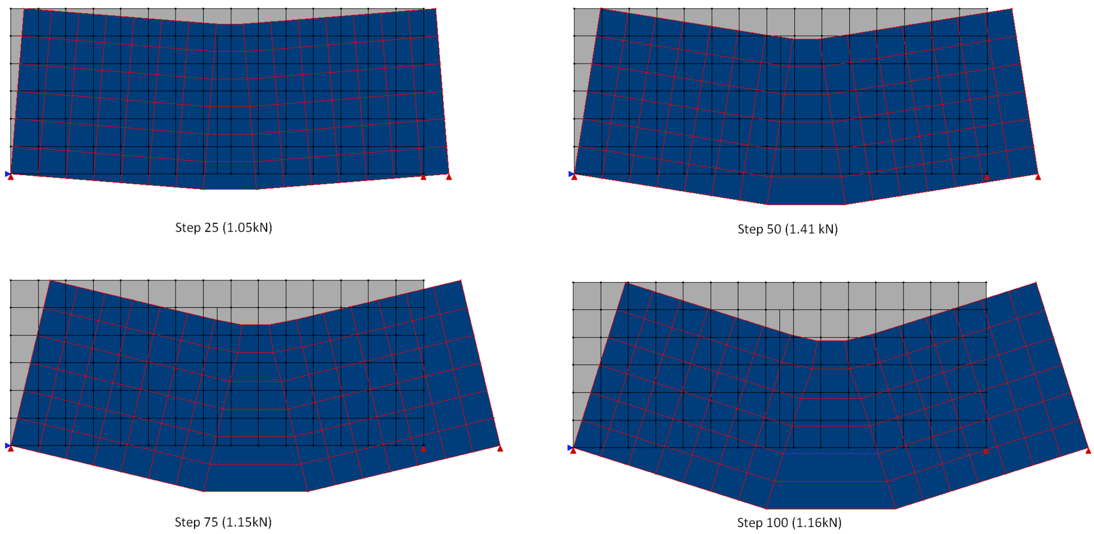


Figure 8. Mesh deformed shape for the steps 25 ($1.05kN$), 50 ($1.41kN$), 75 ($1.15kN$) and 100 ($1.16kN$) of the discontinuity C5

7. FINAL REMARKS

For further research, it is intend to perform the necessary changes on the INSANE numeric core in such way that the discontinuities are introduced during the analysis processing. The discontinuities will be introduced from the identification of the threshold stage of nucleation of cracks, by defining a measure of nucleation. Then, the propagation of the cracks will be taken into account, using GFEM enrichment strategy as well as cohesive laws, governing opening of cracks.

8. ACKNOWLEDGEMENTS

The authors gratefully acknowledge the important support of the Brazilian research agencies CNPq (in Portuguese "Conselho Nacional de Desenvolvimento Científico e Tecnológico" - Grants 486959/2013-9, 309005/2013-2 and 308785 /2014-2) and FAPEMIG (in Portuguese "Fundação de Amparo à Pesquisa do Estado de Minas Gerais" - Grant PPM-00310-13).

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