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NEW DEVELOPMENTS IN THE APPLICATION OF CONFIGURATIONAL MECHANICS TO CRACK PROPAGATION

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Abstract. The numerical description of discrete cracks and their propagation remains one of the main difficulties in the modeling of quasi-brittle materials such as rock or concrete. An emerging powerful approach is the use of Configurational Mechanics concepts, in such a way that crack trajectory really corresponds to a structural energy minimum and is not predetermined by the initial mesh lines. In the implementation developed, discrete cracks, represented by zero-thickness interface elements, are reoriented on the basis of configurational or material forces, calculated in a FEM context by an integration over the elements of the Eshelby energy-momentum tensor. The strategy is illustrated with an application example for which the fracture path is known a priori, and the initial mesh layout is chosen such that the lines zig-zag significantly with respect to it. The results show that the procedure implemented works successfully, that is, mesh lines do succeed in reorienting themselves during configurational iterations, so that the developing crack progressively matches the known physical trajectory.

1 INTRODUCTION

Discontinuities such as cracks or fractures play a fundamental role in the description of mechanical behavior of concrete, rock and other quasi-brittle materials. In the particular cases that the crack trajectory is known a priori (e.g. due to symmetry), accurate numerical descriptions of crack initiation and development may be obtained with the help of Fracture Mechanics principles e.g. using Hillerborg's Fictitious Crack Model [1], or extensions of it via zero-thickness interface elements equipped with appropriate energy-driven constitutive models [2]. In the general case, however, the determination of the crack trajectory itself remains as the main challenge. One solution is to consider all the lines in the mesh as potential crack lines, and let them open/close depending on local stresses [3,4,5]; although this means that cracks can only follow the original mesh lines, which in general may lead to zig-zagging cracks with excessive unrealistic roughness. Alternatively, crack trajectory may be adjusted by modifying the mesh geometry, although the quality of the resulting crack path may be strongly dependent on the criterion used for determining crack orientation. Traditionally, local criteria were used such as direction of maximum tensile stress (e.g. [6]). However, it is well accepted that cracks will develop in the direction that minimizes the global energy of the structure, concept that may be developed and implemented in FE calculations with the help of Configurational Mechanics. The concepts of configurational (or

material) forces and configurational stresses were originally introduced by Eshelby [7]. In the context of the FEM, configurational forces may be understood as derivatives of the global structural energy with respect to the nodal coordinates [8]; thus, as a general idea, moving the nodes in the direction of configurational forces should decrease the global structural energy. Application of the above concepts to mesh optimization and crack propagation has been described in the literature [8-13]. In [14], the authors discussed those concepts with emphasis on the distinction between energy changes due to discretization error ("configurational noise"), and due to physical geometric changes such as dimensions or crack trajectory. In the present paper, recent developments in the application of configurational mechanics to crack propagation are summarized. In the implementation developed, cracks are represented using fracture-based zero-thickness interface elements. During the calculation, configurational forces are evaluated and nodes are relocated to optimize crack trajectory without changing the mesh topology.

2 FEM+Z COMBINED WITH CONFIGURATIONAL MECHANICS

A model based on combining traditional displacement-based FEM including zerothickness interface elements (FEM+z approach), with the contribution of Configurational Mechanics, is proposed to evaluate crack propagation with non-preestablished paths. FEM+z has been extensively used in the past to describe the behavior of fractures with a fixed position, while configurational mechanics provides information on how to move nodes to reorient interface elements when they start cracking, in order to approach a global energy minimum [14].

The FEM+z approach for non-linear fracture analysis is an existing and extensively-tested methodology. It consists of using traditional zero-thickness interface elements [15] in combination with a fracture-based constitutive law [16], while the continuum remains elastic (or visco-elastic) at all times.

In the context of a general, large-strain formulation of the FEM, global elastic energy is a function of original location as well as final node position after deformation \mathbf{x} , i.e. $\psi = \psi(\mathbf{X}, \mathbf{x})$, and configurational nodal forces may be defined as the negative gradient of energy with respect to the original node locations (at constant \mathbf{x}), i.e.:

$$\hat{\mathbf{f}} = -\frac{\partial \psi}{\partial \mathbf{X}} \Big|_{\mathbf{x} = \mathbf{ct}} \tag{1}$$

Developing this equation with standard FE assumptions, configurational nodal forces may be expressed as:

$$\hat{\mathbf{f}} = \int \hat{\mathbf{B}}^T \boldsymbol{\Sigma} \, \mathrm{d} V \tag{2}$$

where $\hat{\mathbf{B}}$ is the non-symmetric version of the traditional "B" FE matrix, and $\boldsymbol{\Sigma}$ is the "configurational stress" given by Eshelby's energy-momentum tensor [8]:

$$\boldsymbol{\Sigma} = \mathbf{W}\mathbf{I} - \mathbf{F}^{\mathrm{T}}\mathbf{P} \tag{3}$$

where W is the elastic energy per unit volume of the undeformed body, \mathbf{F} the deformation gradient and \mathbf{P} the first Piola-Kirchoff stress.

The method implemented basically consists of "moving" the nodes (change their coordinates) by certain magnitude along the directions indicated by configurational forces and, once moved, reevaluate configurational forces and repeat the process iteratively until convergence. Similar to classical deformational analysis, node relocation is subject to some restrictions, such as for instance boundary restrictions not to change the domain geometry.

A peculiarity of zero-thickness interface elements is the presence of double nodes with (generally) the same coordinates. Each pair of nodes may become a cluster of several nodes in the case of interface intersections (Figure 1a). With the purpose of configurational node relocation, all the nodes in a cluser are treated as a single node in a mesh without interfaces (Figure 1b), which is subject to a configurational force equal to the sum of the forces on all the nodes in the cluster.



Figure 1: (a) Standard finite element mesh with zero-thickness interface elements in which all nodes in each cluster have the same coordinates, and (b) equivalent mesh without interfaces.

The simultaneous change of nodal coordinates in all the nodes subject to configurational forces has been shown to desestabilize the process. For this reason, only crack tip nodes are allowed to change their coordinates (Figure 2). Every time interface elements have been reoriented, a "mesh relaxation" algorithm (e.g. [17,18]) is applied to improve mesh quality around the modified area.



Figure 2: Detail of a deformed FE-mesh. The green arrow represents the configurational force $(\hat{\mathbf{f}})$ direction on a crack tip node.

The relocated nodes require a mapping and update of the corresponding nodal variables in order to maintain consistency of the results. This procedure is done by interpolation of the variables in the new position with respect to the previous mesh configuration. The details of this and other auxiliary procedures involved in the implementation are described in [19].

3 NUMERICAL EXAMPLE

A three-point bending beam test of 5x1m is represented in Figure 3. The three-point bending test is a good example to verify simulations of cracking along non-pre-established path because, due to symmetry, it is known that the crack path should be vertical, along the plane of symmetry and starting from the bottom face of the beam. If the process works correctly, the initial zig-zagging mesh lines should get realigned to this vertical crack path.

Deformational boundary conditions consist of nodes at the lower vertices vertically constrained, and a node at the middle of the upper face with horizontal displacements restricted. The loading consists of vertical displacements at this point prescribed with an increasing value (Figure 3).



Figure 3: Boundary conditions of three-point bending test example.

The beam is discretized into triangular elements of quadratic order in order to reduce the discretization error (Figure 4). Due to the expected crack trajectory, and to deal with increasing complexity, interface elements are pre-inserted along a single line zig-zagging around the symmetry line of the beam (red line in Figure 4).

The continuum material is assumed linear elastic (small strain), with Young's modulus of E = 15000MPa and Poisson's ratio v = 0.0.The constitutive model for the interface is the fracture based constitutive model described in [16], with the following parameter values: normal and tangential elastic stiffness $K_N = K_T = 10^7$ MPa/m, friction angle tan $\phi = 0.7$, tensile strength $\chi = 3$ MPa, cohesion c = 6MPa, energy mode I $G^{I_f} = 10^{-2}$ MPa·m, energy mode IIa $G^{IIa}_f = 10^{-1}$ MPa ·m and sigma dilatation $\sigma_{dil} = 30$ MPa.



Figure 4: Initial configuration of beam bending realignment.



Figure 5: Final configuration of beam bending realignment.



Figure 6: Three-point bending test deformation after solving the deformational and configurational problem (displacement magnification x100).

As Figure 6 depicts, the crack is initiated at the center of the lower face of the beam and propagates upwards. In Figures 5 and 6 the final state of the beam is depicted. These figures show that the iterative configurational process succeeds in orienting the crack along the correct vertical direction.

In the figures, red lines correspond to the zero-thickness interface elements which have not started cracking yet, and therefore, in the scheme implemented they have not triggered the process of moving nodes (although some of them may have changed orientation if they share nodes with an interface which has started cracking, such is the case of the top interface in Figures 5 and 6). Blue lines correspond to the interface elements that have started cracking, and therefore configurational forces may have moved them to an optimal position.

Figure 7 displays two load-displacement curves, the one obtained for the initial configuration fixed (mesh with the distorted crack trajectory), and the other one obtained after crack realignment (solving the FEM problem with the final configuration, mesh with the vertical crack path). As it could be expected, the load-displacement curve obtained from the final configuration exhibits a lower, more realistic peak and post-peak response. This is because in the final configuration interface elements are better oriented and therefore the crack initiates and propagates with lower applied load values.



Figure 7: Three-point bending test load-displacement curves.

4 CONCLUDING REMARKS

This article is focused on describing discrete cracks with traditional zero-thickness interface elements of initial random orientation, and obtaining their correct orientation for crack propagation on the basis of concepts of configurational mechanics. In the FEM context, configurational nodal forces indicate the direction in which nodal coordinates should be changed to minimize global energy. An iterative process based on this idea leads to progressive reorientation of interface elements as cracks open and propagate. An example of application consisting of a three-point bending beam shows that the approach proposed succeeds in re-orienting the initially random mesh into a well-aligned crack developing along the symmetry plane of the beam.

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