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APPLICATION OF CONFIGURATIONAL MECHANICS TO CRACK PROPAGATION

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Abstract. Crack initiation and propagation is an essential aspect in the mechanical behavior of a large variety of materials and structures in all fields of Engineering and, in particular, the prediction of crack trajectories is one of the major challenges of existing numerical methods. Classical procedures to fix crack direction have been based on local criteria such as maximum (tensile) hope stress. However, Fracture Mechanics principles suggest that global criteria should be used instead, such as maximizing structural energy release rates. An emerging trend along this way is based on Configurational Mechanics, which describes a dual version of the mechanical problem in terms of configurational pseudo-stresses, pseudo-forces, etc. all with a physical meaning related to the change in global structural elastic energy caused by changes in the structural geometry (configuration). In the FEM context, these concepts are applied to optimize the total energy of the mesh with respect to reference coordinates using the discrete configurational forces. Configurational stresses given by Eshelby's energy-momentum tensor may be integrated using standard expressions to give configurational nodal forces. Adequate treatment of these forces in the context of iterative FE calculations, may lead to prediction of crack trajectories in terms of global structural energy.

1 INTRODUCTION

The purpose of this paper is to introduce basic ideas of Configurational Mechanics related to crack initiation and propagation. According to Steinmann [1], Configurational Mechanics can be considered from the viewpoints of continuum mechanics or computational mechanics. In the context of continuum mechanics, configurational forces would describe the energy variations due to changes of material configuration, while in a computational context the discrete forces may indicate the quality of a finite element mesh. In both cases, configurational analysis consists of evaluating the energy variations due to changes of the material configuration (original geometry of the structure or mesh). Configurational mechanics may be used to solve a large variety of problems, such is mechanics of dielectrics, thermodynamic problems, or mechanical problems with presence of dislocations and fractures, etc.

Configurational forces are derived combining the energy and momentum balance, with the so called pseudo-momentum balance or configurational force balance. The original concept is due to Eshelby [2], who introduced the so called energy-momentum tensor $\boldsymbol{\Sigma} = \mathrm{W}\mathbf{I} - \mathbf{F}^{\mathrm{T}}\mathbf{P}$. In the fifties, Eshelby developed the driving forces for elastic singularities, defining the well-known "Maxwell tensor of elasticity". Configurational forces are the negative gradient of total energy with respect to the position of a point or defect, so forces are used to evaluate imperfections, dislocations, etc.

In addition, configurational forces may take a special meaning in the context of the Finite Element Method, because the FEM yields only approximate solutions which depend on discretization. The equilibrium equation is approximated but not exactly satisfied, and energy is also approximated but not exactly evaluated, and the error may depend on the chosen discretization. The concept of finite element mesh optimization using configurational forces is described in [1, 3, 4, 5, 6, 7], with application to remeshing methods or r-adaptivity methods [3, 7].

2 CONFIGURATIONAL MECHANICS IN THE CONTEXT OF THE FINITE ELEMENT METHOD

Configurational forces show the direction in which the original position of the nodes of mesh would have to be moved, so that the overall energy in the mesh would decrease. Energy variation can be caused by physical changes such as changes in dimensions of geometry of the domain (if the nodes changing location are at the boundary for instance), or changes of the mesh discretization (if the nodes changing location are in the interior of the domain and their location does not affect the boundaries but only the internal arrangement of the mesh).

Nevertheless, both can be represented by configurational forces which are the gradient of the total domain elastic energy ψ with respect to original nodal location $\mathbf{X}$ (Eq. 1). Since, in general, energy is a function of original location as well as final node position after deformation $\mathbf{x}$, i.e. $\psi = \psi(\mathbf{X}, \mathbf{x})$, this means that configurational forces are evaluated at constant $\mathbf{x}$:

$$\hat{\mathbf{f}} = \left.\frac{\partial \psi}{\partial \mathbf{X}}\right|_{\mathbf{x}=\mathbf{ct}} \tag{1}$$

In the finite element context, energy may be expressed as an integral over the domain, of the specific energy per unit volume, which leads to the following integral expression of the configurational forces:

$$\hat{\mathbf{f}} = \int \mathbf{B}^{T}(\mathrm{W}\mathbf{I} - \mathbf{F}^{\mathrm{T}}\mathbf{P})\mathrm{dV} \tag{2}$$

where **B** is the traditional FE matrix, W is the specific elastic energy per unit volume of original configuration, **I** is the 3x3 unit matrix, **F** is the deformation gradient and **P** is the first Piola-Kirchoff stress.

Equation (2) may be obtained by combining the basic definition of configurational forces (Eq.1) with finite element equations, or by alternative procedures as it is developed in some articles [4, 5, 6, 7].

Expression (2) contains the well-known Eshelby's stress tensor, also called energy-momentum tensor, which is defined as:

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

Note the alternative expression of $\boldsymbol{\Sigma}$ in terms of symmetric tensors, second Piola-Kirchhoff ($\mathbf{S} = \mathbf{F}^{-1}\mathbf{P}$) and symmetric right Cauchy-Green strain tensor ($\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$).

Notice that the definition of configurational forces is similar to mechanical forces in the classical (deformational) finite element formulation. In this case, instead of the physical stress the integral is over shape function derivatives and the Eshelby's stress tensor.

$$\mathbf{f} = \int \mathbf{B}^T \boldsymbol{\sigma}\, dV \;\rightarrow\; \hat{\mathbf{f}} = \int \mathbf{B}^T \boldsymbol{\Sigma}\, dV \tag{4}$$

As said, configurational forces indicate the direction in which nodes should be configurationally moved (original coordinates changed) in order to decrease the overall domain elastic energy, and eventually reach the minimal energy configuration. On the basis of that, an r-adaptivity method has been implemented. It is an iterative process which consists of changing nodal location until material forces vanish. The change of location for each iteration is calculated via Eq.(5), using a small value for constant c multiplying the configurational forces with minus sign (logical, since being those forces the gradient of the energy, their positive direction would indicate energy increase):

$$\mathrm{X}_i = \mathrm{X}_{i-1} - c\hat{f}_{i-1} \tag{5}$$

In this equation, X are the nodal coordinates, $\hat{f}$ the configurational forces and subindex i indicates the current configurational iteration.

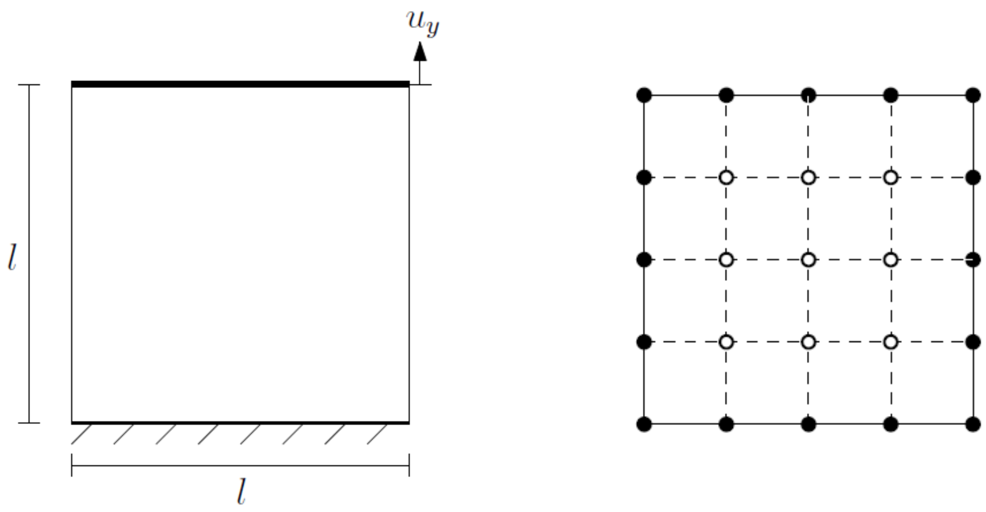
The r-adaptivity procedure provides energetically optimized meshes, where number of elements remains constant and connectivity as well. These may be great advantages in comparison to other more complex methods such as h-adaptivity methods [7].

3 NUMERICAL EXAMPLES

3.1 Example 1

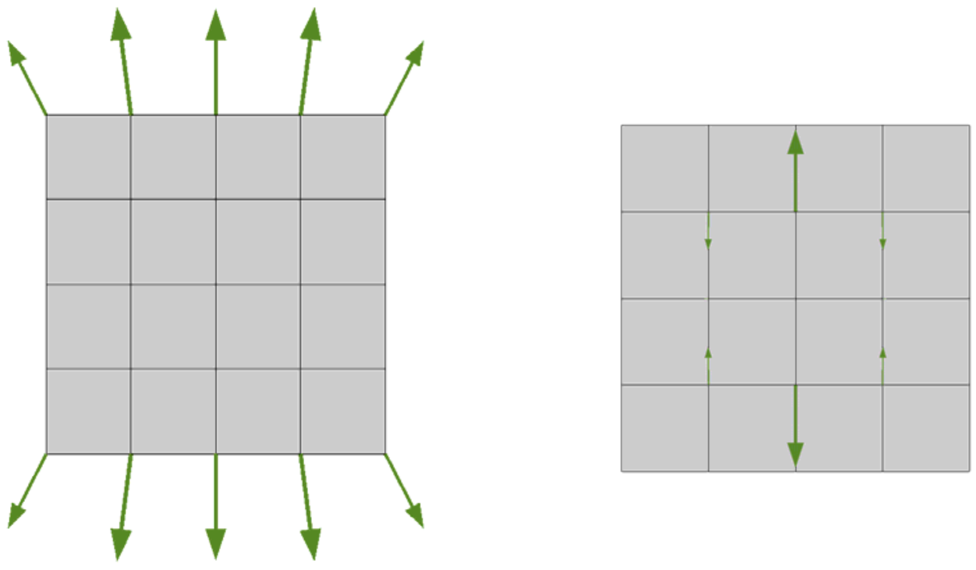
This example has been often used in configurational mechanics papers [4]. It consists on a homogeneous block (E=1085.7 MPa and ν =0.3571) with a constrained tensile displacement on the top side and fixed on the bottom (Figure 1a). It is discretized with a structured mesh of 16 regular quadrilateral elements as shown in Figure 1b, where the solid nodes also indicate the nodes that are "configurationally fixed" (i.e. those that will not be allowed to move even if configurational forces are applied on them), while the hollow ones are "configurationally free" to change location through configurational iterations.

In this problem, configurational forces (with minus sign) are concentrated on the boundary nodes that are configurationally fixed (Figure 2a), with such proportion that if scale is adjusted to those, the forces on inner nodes cannot be even visualized. Physically this means that, if domain dimensions would be increased slightly (but final node positions would remain constant), total energy would decrease. To explain this, one has to take into account two counteracting effects. On one side, tensile deformations would be lower (because initial and final positions of nodes would be closer) and therefore volumetric energy density would be lower, but on the other side total volume would be larger. Out of those effects, the decrease of specific energy would be dominant because is a quadratic relation. From the r-adaptivity method itself, it makes sense to fix configurational movements on the boundary so that domain dimensions will not change and only internal configurational forces (Figure 2b) are allowed to change the material configuration, and therefore node relocations will reflect only the mesh rearrangement to reach an energy minimum



(a) (b)

Figure 1: (a) Boundary conditions of example 1 (b) Finite element discretization, with indication of nodes that are "configurationally fixed" (solid) and "configurationally free" (hollow).



(a) (b)

Figure 2: (a) Configurational forces (with minus sign) on all nodes of the mesh, at the scale dictated by larger forces on the boundary nodes, (b) same only for internal nodes, at a larger scale in which forces on those nodes would be represented.

Finally, applying equation (5) in various steps with an appropriate value of c leads to the optimized mesh. As Figure 3a shows, nodes with larger configurational forces exhibit larger position changes. Since this optimal corresponds, not to a real geometry change of the domain but to the optimization of the FE discretization error, this solution turns out not trivial and might be different for other meshes or element types. Figure 3b depicts the total energy of the mesh as a function of the y-coordinate position of the most relevant node in this example, and Figure 3c the norm of the configurational forces of internal nodes, also as a function of the same vertical position of the relevant node. It can be seen as the node approaches it optimal position, energy comes to a minimum and forces are reduced to zero norm.

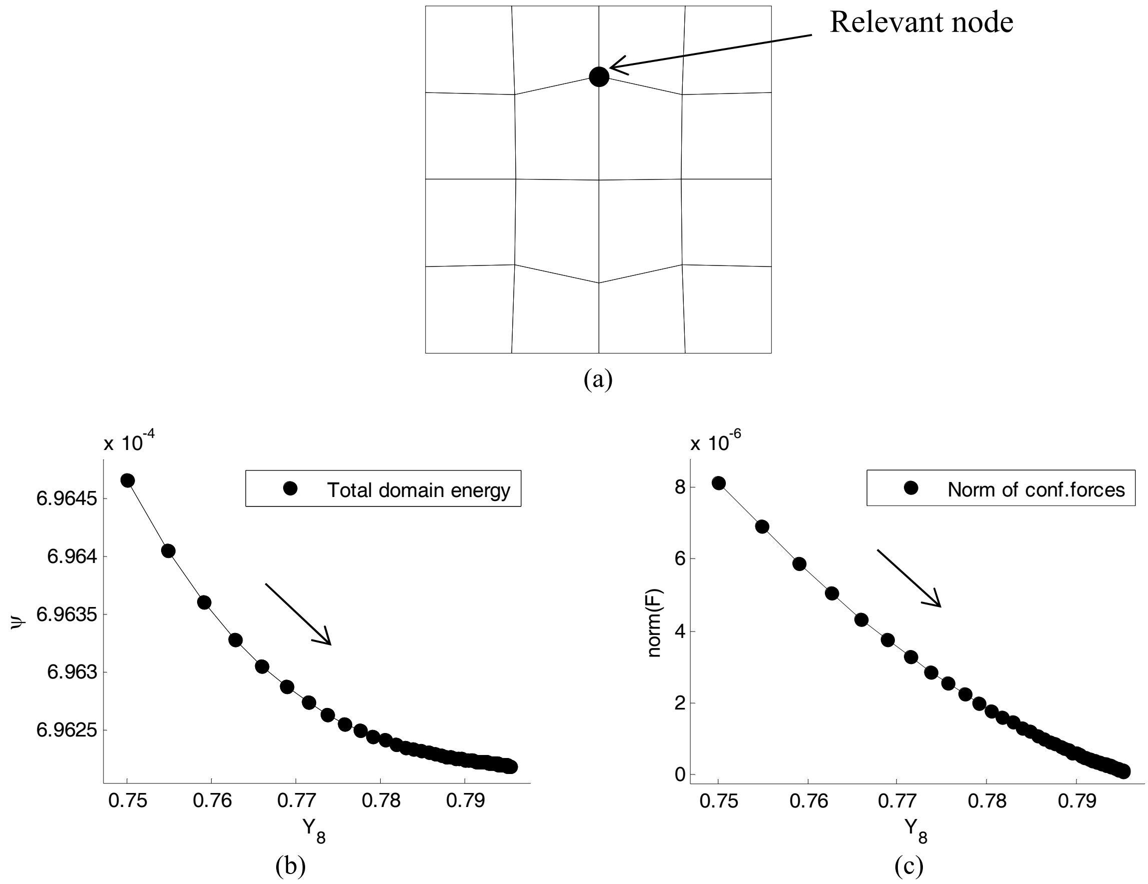


Figure 3: (a) Optimal mesh configuration. (b) Total mesh energy with respect to relevant node vertical position, and (c) norm of configurational forces with respect to relevant node vertical position.

3.2 Example 2

The second example is a notched beam with a prescribed displacement on the top. In this case the point where displacement is imposed is not aligned with the notch, in order to observe the path followed by the central top node of the notch (Figure 4). Material properties are $\lambda = 1000$, $\mu = 400$ (Lamé Constants, which correspond to E=1085.7 MPa and ν =0.3571) and plane strain is assumed.

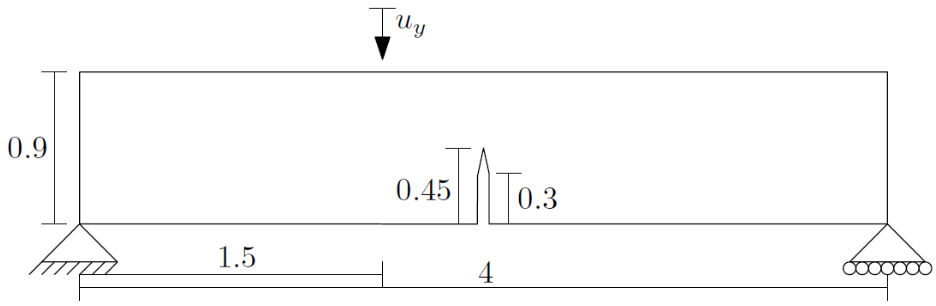


Figure 4: Notched beam on two supports with a punctual displacement imposed on the top.

The mesh discretization used to analyze path evolution in vertical and horizontal direction is shown in Figure 5, there are six quadrangular elements. The advantage of using that simple structure is is that only one node is not configurationally fixed, and therefore it is easier to understand energy distribution and configurational force effects depending on its position.

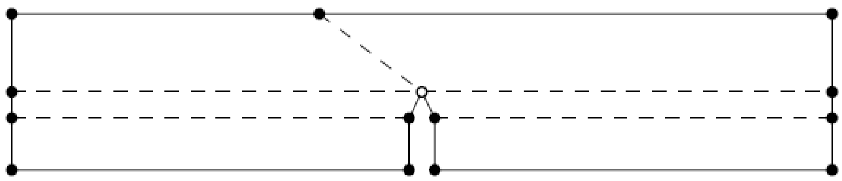


Figure 5: Finite element mesh used on example 2.

As the interactive procedure starts, configurational forces drive the central node progressively to its optimal energetic position. As it is represented in Figure 8a, the optimal position is at the point of coordinates X = 1.5 and Y = 0.9, which is the application point of the imposed displacement. Figures 6, 7 and 8 confirm that solution because there is a minimum of energy and the norm of configurational forces are near zero at the point X = 1.5 and Y = 0.9.

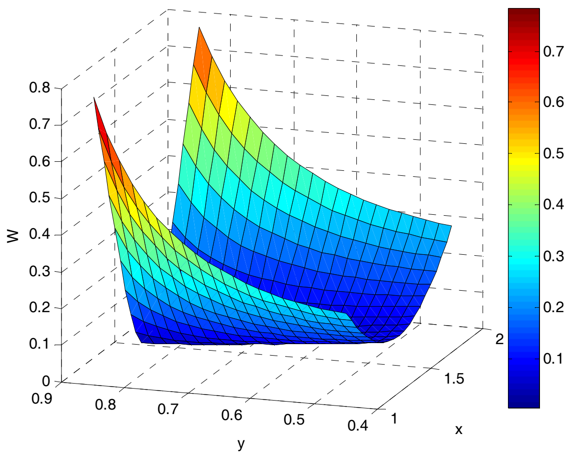


Figure 6: Total domain energy as a function of the central node position.

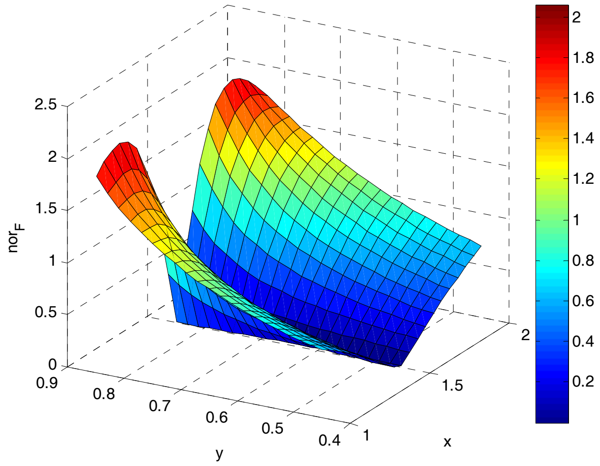
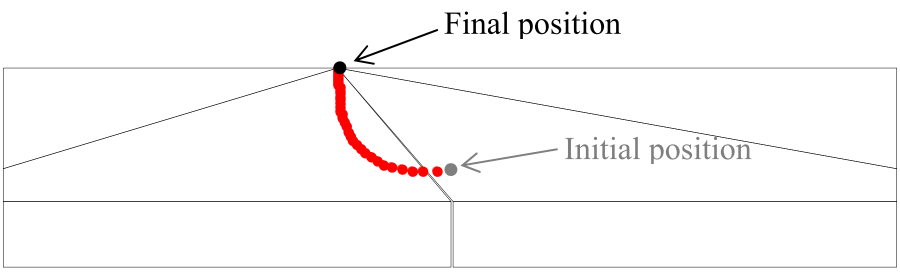
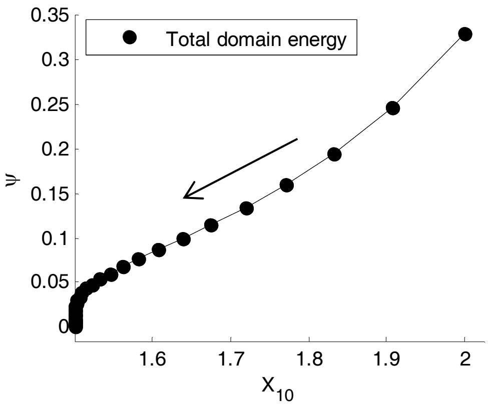


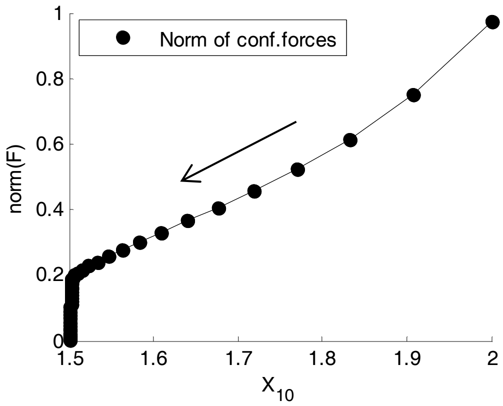
Figure 7: Configurational force norm as a function of the central node position.



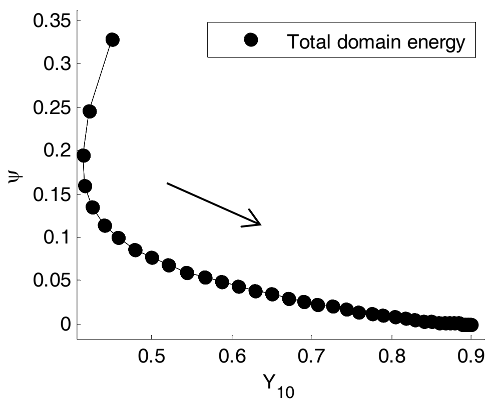
(a)



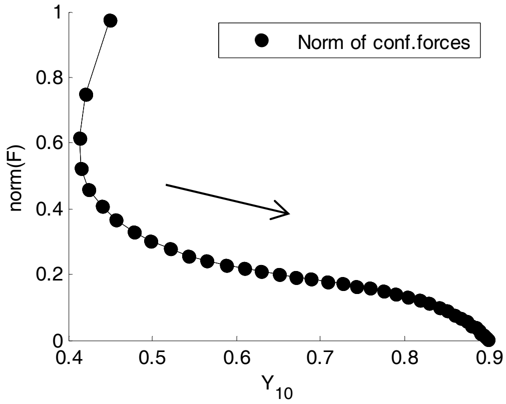
(b)



(c)



(d)



(e)

Figure 8: (a) Optimal mesh distribution, the path is represented in red. (b) Total energy with respect to the relevant node horizontal position. (c) Norm of configurational forces with respect to the relevant node horizontal position. (d) Total energy with respect to the relevant node vertical position. (e) Norm of configurational forces with respect to the relevant node vertical position.

4 CONCLUDING REMARKS

In this article the application of configurational mechanics to FE meshes has been introduced. Configurational forces are used to know the direction in which the nodes original positions would have to be moved, in order to decrease the total domain energy and eventually reach the minimum energy configuration. Using this concept as an r-adaptive strategy, nodal coordinates may be modified leading to the optimal mesh (in the energy sense). From a physical point of view, configurational forces may also be used to indicate the direction of crack tip propagation for minimal energy and therefore help predict the most probable path on crack trajectories. In example 1, a simple mesh optimization was performed reaching the minimum total energy for some non-trivial configuration. On the other hand, the second example was useful to illustrate how configurational forces can be applied to evaluate optimal crack paths. Note that in this academic example the notch was allowed to move (and therefore the crack could grow) without restrictions or energy consumption, only driven by configurational forces exclusively, that is only responding to the direction of crack extension that will reduce more effectively the total energy of the domain. This is why, the minimum is reached for zero total energy, when the crack tip arrives to the point of prescribed displacement, configuration that actually corresponds to a hinge mechanism. But physically, crack extension requires energy consumption. And this is precisely one of the focus of on-going work, complementing configurational mechanics with the restrictions imposed by the principles of fracture mechanics that dictate the balance between energy released from the structure and energy consumption required for crack propagation.

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