

A TOPOLOGICAL DERIVATIVE-BASED HYDRAULIC FRACTURE MODEL IN BRITTLE MATERIALS

M. XAVIER, N. VAN GOETHEM AND A.A. NOVOTNY

ABSTRACT. This paper deals with a novel hydraulic fracture model based on the concept of topological derivative. The basic idea consists in adapting the Francfort-Marigo damage model to the context of hydraulic fracture. The Francfort-Marigo damage model is a variational approach to describe the behavior of brittle materials under the quasi-static loading assumption, focusing on the evolution of damage regions under an irreversibility constraint. In our problem, the loading comes out from a prescribed pressure acting within the damage region, which is used to trigger the hydraulic fracturing process. A shape functional given by the sum of the total potential energy of the system with a Griffith-type dissipation energy term is minimized with respect to a set of ball-shaped pressurized inclusions by using the topological derivative concept. In particular, the topological asymptotic expansion of the shape functional with respect to the nucleation of a circular inclusion endowed with non-homogeneous transmission condition on its boundary is rigorously developed. The associated topological derivative, which corroborates with the famous Eshelby theorem, is used to devise a simple topology optimization algorithm specifically designed to simulate the whole nucleation and propagation process of hydraulic fracturing. To assess our model, some numerical examples are presented, showing typical features of hydraulic fracture phenomenon, including the characterization of the fault-activation pressure and specific crack path growth, allowing for kinking and bifurcations.

1. INTRODUCTION

Hydraulic fracturing is an industrial process that requires to pump a mixture of water, proppant (usually sand), and some chemical additives into layers of rock and shale. The purpose is to create and/or extend cracks from some pre-existing geological faults in order to let the gas that was trapped into the rocks be extracted at the surface. Roughly speaking, the process starts by perforating a vertical well into the reservoir. As soon as the required depth is reached, the perforation continues in the horizontal direction. Finally, the pumping mechanism of the aforementioned mixture at an extremely high pressure is launched. Then, the pressure inside the damaged region is increased until a critical value is attained at which fault-activation is triggered.

In order to study the hydraulic fracturing process, we consider an idealized reservoir composed by the horizontal pressurization well within the region to be fractured. It is supposed that the fracture pattern is periodic. Therefore, adopting convenient boundary conditions, it is sufficient to consider a single block as reference domain to represent the whole fracture network. See sketch in Figure 1.

In particular, this paper deals with a novel hydraulic fracture model based on the topological derivative concept. The basic idea consists in adapting the Francfort-Marigo damage model [8] to the context of hydraulic fracturing phenomenon. The Francfort-Marigo damage model describes the behavior of brittle materials under the quasi-static loading assumption, focusing on the evolution of damage regions under an irreversibility constraint. Such a model has been successfully applied to simulate fracturing process in brittle materials, where the crack is identified with a thin damage [4, 5]. See also recent

Date: June 12, 2017.

Key words and phrases. Topological Derivative, Hydraulic Fracture Model, Topology Optimization Algorithm.

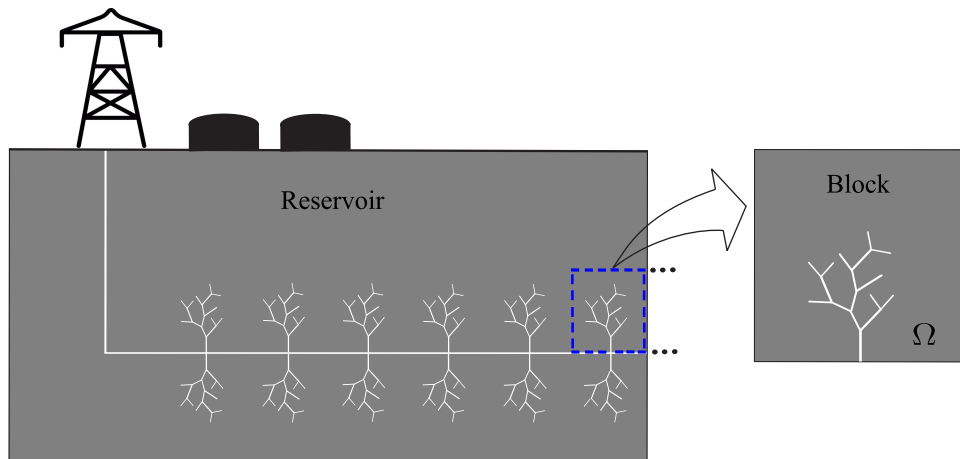


FIGURE 1. Fractured reservoir.

papers [1, 18] where the topological derivative concept is incorporated to the Francfort-Marigo model. In the context of the problem we are dealing with, the loading comes out from a prescribed pressure inside the damaged region, which is used to trigger the hydraulic fracturing process. Thus, a shape functional given by the sum of the total potential energy of the system with a Griffith-type dissipation energy term is minimized with respect to a set of ball-shaped pressurized inclusions by using the topological derivative concept [14, 16]. More precisely, the topological asymptotic expansion of the shape functional, taking into account the nucleation of a circular inclusion endowed with non-homogeneous transmission condition on its boundary, is rigorously developed. It is observed that the obtained topological derivative fits the famous Eshelby theorem [6, 7] which represents one of the major advances in the continuum mechanics theory of the 20th century [11]. The associated topological derivative is used as descent direction to minimize the proposed shape functional indicating the regions that have to be damaged. Based on this natural idea, a simple topology optimization algorithm specifically designed to simulate the whole nucleation and propagation hydraulic fracturing process is devised. Finally, some numerical examples are presented, showing important features associated with hydraulic fracture phenomenon, including the characterization of the fault-activation pressure and crack path growth, allowing for kinking and bifurcations.

The hydraulic fracturing process is nowadays very much debated, since in its current form it is extremely damageable for the ecosystem. In particular, it is currently forbidden in Europe and many regions of the world, including Brazil, since an uncontrolled use of this technique leads to severe environmental issues. The first is water consumption: in 2010, the U.S. Environmental Protection Agency estimated that 300 to 500 million cubic meters of water are used to fracture 35.000 wells in the United States each year. The extraction of so much water for fracking has raised concerns about the ecological impacts to aquatic resources, as well as dewatering of drinking water aquifers. A second dramatic issue is the fact that shale gas wells can use more than 2 million kilograms of proppant per well, that is, about 5 times more than alternative oil extraction techniques. Furthermore, in addition to large volumes of water, a variety of chemicals are used in hydraulic fracturing fluids, typically of the order of 0.5% and 2.0% of the total volume of the fracturing fluid, which represents huge quantities in respect of the enormous volume of water used¹.

¹see https://www.earthworksaction.org/issues/detail/hydraulic_fracturing_101#.WRluRDe1tpg

It is therefore of major importance to be able to numerically simulate any such shale gas extraction technique, in order to anticipate the risks, monitorate and optimize the industrial process. Many models have been proposed over the years but they are either too simplified or they tend to focus on one key aspect of fracking (see, e.g. the survey [10]). Moreover, the scarcity of in-situ data makes the study of fracking even more complicated. To the knowledge of the authors, alternative approaches rely on nonlinear fracture mechanics models, with *ad-hoc* nucleation and propagation laws, as documented in [10]. See also [19]. Therefore, our approach which is linear and purely variational shows the advantage of being simple and easily implemented, as well as grounded by solid mathematical basis. Our aim is also to provide some benchmarks to allow comparison with other methods, since very few numerical data is currently available.

The paper is organized as follows. The hydraulic fracture mechanical model is presented in Section 2. The existence of the associated topological derivative is proved in Section 3, where its closed form is rigorously derived. In Section 4 the resulting topology optimization algorithm is presented in details. A set of numerical experiments are driven in Section 5. Finally, some concluding remarks are presented in Section 6.

2. HYDRAULIC FRACTURE MODEL

In this section we present the main aspects concerning Francfort-Marigo damage model together with its adapted version to the context of hydraulic fracture phenomenon.

2.1. Francfort-Marigo damage model. Damage models, like the one introduced by Francfort-Marigo, initially propose that a damaged elastic body is composed by two distinct materials. To introduce this idea, let us consider an open and bounded domain $\Omega \subset \mathbb{R}^2$ with Lipschitz boundary $\partial\Omega$ and a sub-domain ω of the form $\omega \subset \Omega$, see Figure 2. Then, a parameter ρ , defined as

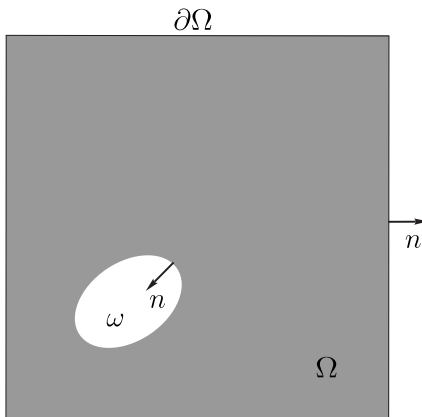


FIGURE 2. Unperturbed problem.

$$\rho = \rho(x) := \begin{cases} 1, & \text{if } x \in \Omega \setminus \bar{\omega}, \\ \rho_0, & \text{if } x \in \omega, \end{cases} \quad (2.1)$$

with $0 < \rho_0 \ll 1$, is introduced to characterize the damage distribution. Therefore, the region $\Omega \setminus \bar{\omega}$ represents the healthy part of the domain, while ω represents the damaged region.

The change from the original material to the damaged one occurs only if the elastic energy released by this transition overcomes a certain material-dependent threshold. In

other words, the occurrence of new damage is determined by the relation

$$\frac{1}{2}\mathbb{C}\epsilon \cdot \epsilon - \frac{1}{2}\rho_0\mathbb{C}\epsilon \cdot \epsilon > \kappa, \quad (2.2)$$

where \mathbb{C} is the fourth-order elasticity tensor, ϵ is the second-order strain tensor and κ is a material property that represents the damage toughness.

Finally, the model proposes a shape functional, $\mathcal{F}_\omega(u_i)$, to be minimized at each time step t_i , defined as

$$\mathcal{F}_\omega(u_i) = \mathcal{J}(u_i) + \kappa|\omega|, \quad (2.3)$$

where u_i is the displacement field at the time t_i and $|\omega|$ is the Lebesgue measure of ω . As mentioned, the first term on the right side of (2.3) represents the total potential energy of the system while the second term is the so called Griffith-type dissipation energy.

In addition, two conditions are assumed in this model. The first one considers that the healthy material should be stiffer than the damaged phase to characterize the stiffness loss associated to the crack growth. The second condition ensures that the fracturing process is irreversible, which means that healing is precluded. For a complete description of the Francfort-Marigo damage model see the original paper [8].

2.2. Mechanical model for hydraulic fracture. Now, in order to adapt the Francfort-Marigo model to the context of hydraulic fracture it is considered that the damaged region ω is submitted to some internal pressure. By this way, a normal force is applied on the damage front $\partial\omega$. In addition, the pressure inside the damaged region ω , depending on the time instant t_i , is given by

$$p_i = p_{i-1} + \Delta p_i \quad (2.4)$$

where Δp_i is the pressure increment. Therefore, the total applied pressure p is computed as the sum

$$p = p_0 + \sum_{i=1}^N \Delta p_i, \quad (2.5)$$

where p_0 is the initial pressure and N the total number of increments. Note that for each incremental pressure p_i a new displacement field u_i is induced. Then, in order to simplify future notations the subscript i in the displacement field u_i will be omitted.

Therefore, the hydraulic fracture model has the same structure of Francfort-Marigo model and, in particular, relies on the following shape functional:

$$\mathcal{F}_\omega(u) = \mathcal{J}(u) + \kappa|\omega|, \quad (2.6)$$

where the total potential energy $\mathcal{J}(u)$ is given by

$$\mathcal{J}(u) = \frac{1}{2} \int_{\Omega} \sigma(u) \cdot \nabla u^s dx - \int_{\omega} p_i \operatorname{div}(u) dx. \quad (2.7)$$

where p_i is the current pressure assumed to be constant in $\omega \subset \Omega$. The vector function u is solution to the following variational problem: Find $u \in \mathcal{U}$, such that

$$\int_{\Omega} \sigma(u) \cdot \nabla \eta^s dx = \int_{\omega} p_i \operatorname{div}(\eta) dx, \quad \forall \eta \in \mathcal{V}. \quad (2.8)$$

Some terms in the above variational equation require explanation. The stress tensor $\sigma(\varphi)$ is given by

$$\sigma(\varphi) = \rho\mathbb{C}\nabla\varphi^s, \quad (2.9)$$

where the parameter ρ is given by (2.1). We consider isotropic material, so that the elasticity tensor \mathbb{C} can be represented by the Lamé's coefficients μ and λ in the following form:

$$\mathbb{C} = 2\mu\mathbb{I} + \lambda(\mathbf{I} \otimes \mathbf{I}), \quad (2.10)$$

where \mathbf{I} and \mathbb{I} are the second and fourth order identity tensors, respectively. The strain tensor $\nabla\varphi^s$ is given by the symmetric part of the gradient of φ , namely

$$\nabla\varphi^s = \frac{1}{2}(\nabla\varphi + (\nabla\varphi)^\top). \quad (2.11)$$

The set \mathcal{U} and the space \mathcal{V} are defined as:

$$\mathcal{V} := \mathcal{U} := H_0^1(\Omega). \quad (2.12)$$

The strong formulation associated with the variational problem (2.8) is given by: Find u , such that:

$$\left\{ \begin{array}{ll} \operatorname{div}\sigma(u) = 0 & \text{in } \Omega, \\ \sigma(u) = \rho\mathbb{C}\nabla u^s, & \\ u = 0 & \text{on } \partial\Omega, \\ \begin{array}{l} \llbracket u \rrbracket = 0 \\ \llbracket \sigma(u) \rrbracket n = -p_i n \end{array} & \text{on } \partial\omega \end{array} \right\} \quad (2.13)$$

where the operator $\llbracket \varphi \rrbracket$ is used to denote the jump of the function φ on the interface $\partial\omega$, namely $\llbracket \varphi \rrbracket = \varphi|_\Omega - \varphi|_\omega$ on $\partial\omega$. The transmission condition on the interface $\partial\omega$ comes out from the variational formulation (2.8).

As can be seen, the hydraulic fracture model is a simple extension of the Francfort-Marigo damage model. Thus, the damage evolution is based just on the energy density distribution. One well-known limitation is that this kind of models are not able to distinguish between traction and compression stress states, so that some phenomena, such as crack closure or lips interpenetration for example, cannot be captured. However the mechanism of hydraulic fracturing is such that these drawbacks do not apply, being the crack opening purely of traction-type, i.e., the crack faces are forced to move away.

Remark 1. *Note that, from the superposition principle, the actions of body forces and the pressure can be treated separately. In the present work we are focusing on the influence of the internal pressure only. In other words, in this work we are considering the main technical problem out of the complete hydraulic fracturing process.*

2.3. Statement of the optimization problem. The minimization problem we are dealing with can be defined in the following way: for each time increment t_i ,

$$\underset{\omega \subset \Omega}{\text{Minimize}} \mathcal{F}_\omega(u), \text{ subject to (2.8)}, \quad (2.14)$$

where $\mathcal{F}_\omega(u)$ is given by (2.6).

A natural approach to deal with such a minimization problem consists in appealing to the topological derivative concept. The basic idea consists in evaluating the topological derivative of the shape functional (2.6) with respect to the nucleation of a small circular pressurized inclusion. Then, the associated topological derivative can be used as a descent direction to solve the minimization problem (2.14) indicating, at each iteration, the regions that have to be damaged.

In the context of hydraulic fracture, the fault-activation pressure is the specific value of the pressure at which activation of the geological fault takes place. An important feature associated with the proposed hydraulic fracture model concerns the characterization of such a critical pressure. The difficulty to deal with problems with stress singularities by using Francfort-Marigo's model is that the strain energy density rises locally to unbounded

values at the crack tip and consequently above any finite threshold. Nevertheless, experiments like those of Griffith indicate the existence of a critical nonzero load even in the presence of such singularities, which reveals a limitation on the straightforward application of the Francfort-Marigo's model in these cases. Note that in the case of damage this singularity is not observed. As a matter of fact, the same difficulty is observed to characterize the critical pressure in the context of hydraulic fracture phenomenon. In this sense, it is necessary to verify by some numerical strategy if the hydraulic fracture model permits the characterization of such a critical pressure. There exists some remedies available in the literature to bypass this problem, see for instance [1]. We are adopting here the same strategy proposed in [18]. The idea consists in introducing a new material property κ_s used together with a scaling factor given by the width δ of the initial damage. In particular, we replace κ by a modified energy release parameter κ_δ defined as

$$\kappa = \kappa_\delta := \frac{\kappa_s}{\delta}. \quad (2.15)$$

From the physical point of view, when δ becomes smaller, the parameter κ_δ increases in a similar way as the energy density, so that the critical pressure converges to a finite nonzero value. This strategy has shown to be effective in problems of crack propagation where the fracture is represented by a damaged region of small width δ , since letting $\delta \rightarrow 0$ forces the damage region to be crack-like.

Remark 2. *In the original Bourdin, Francfort and Marigo work [5], the crack was approximated by a smeared region by Ambrosio and Tortorelli functional [2], whereas in our model the contrary is done: a damage converges to a crack. In the anti-plane case theoretical results in this respect were derived by Dal Maso and Iurlano [13]. Note the use of κ_s is explicitly taken into account in these approximations. See also [12], where a phenomenological continuum model for mode III dynamic fracture based on the phase-field approach is proposed.*

3. TOPOLOGICAL SENSITIVITY ANALYSIS

The topological sensitivity analysis provides a scalar field, called topological derivative, that represents the first order correction of the topological asymptotic expansion of a given shape functional with respect to the introduction of infinitesimal perturbations such as holes, inclusions, source terms or cracks. In other words, the topological derivative measures the sensitivity of the shape functional with respect to the introduction of topological perturbation.

Let us consider an open and bounded domain $\Omega \subset \mathbb{R}^2$ with a Lipschitz boundary $\partial\Omega$, which is subject to a nonsmooth perturbation confined in a small region $B_\varepsilon(\hat{x})$ of size ε centered at an arbitrary point $\hat{x} \in \Omega$, as sketched in Figure 3. We introduce a characteristic function $x \mapsto \chi(x)$, $x \in \mathbb{R}^2$, associated with the unperturbed domain, namely $\chi = \mathbf{1}_\Omega$, such that:

$$|\Omega| = \int_{\mathbb{R}^2} \chi(x) dx, \quad (3.1)$$

where $|\Omega|$ is the Lebesgue's measure of Ω . Then, we define a characteristic function associated with the topologically perturbed domain of the form $x \mapsto \chi_\varepsilon(\hat{x}; x)$, $x \in \mathbb{R}^2$. In the case of a perforation, for example, $\chi_\varepsilon(\hat{x}) = \mathbf{1}_\Omega - \mathbf{1}_{B_\varepsilon(\hat{x})}$, the perforated domain is obtained as $\Omega_\varepsilon(\hat{x}) = \Omega \setminus \overline{B_\varepsilon(\hat{x})}$. Then, we assume that a given shape functional $\psi(\chi_\varepsilon(\hat{x}))$, associated with the topologically perturbed domain, admits the following topological asymptotic expansion:

$$\psi(\chi_\varepsilon(\hat{x})) = \psi(\chi) + f(\varepsilon)D_T\psi(\hat{x}) + o(f(\varepsilon)), \quad (3.2)$$

where $\psi(\chi)$ is the shape functional associated to the original domain, that is, without perturbation, $f(\varepsilon)$ is a positive function such that $f(\varepsilon) \rightarrow 0$ when $\varepsilon \rightarrow 0$ and $o(f(\varepsilon))$ is the remainder. The function $\hat{x} \mapsto D_T\psi(\hat{x})$ is called the topological derivative of ψ at \hat{x} . Therefore, this derivative can be seen as a first order correction of $\psi(\chi_\varepsilon(\hat{x}))$. In fact, after rearranging (3.2) we have

$$\frac{\psi(\chi_\varepsilon(\hat{x})) - \psi(\chi)}{f(\varepsilon)} = D_T\psi(\hat{x}) + \frac{o(f(\varepsilon))}{f(\varepsilon)}. \quad (3.3)$$

The limit $\varepsilon \rightarrow 0$ in the above expression leads to the general definition for the topological derivative, namely

$$D_T\psi(\hat{x}) = \lim_{\varepsilon \rightarrow 0} \frac{\psi(\chi_\varepsilon(\hat{x})) - \psi(\chi(x))}{f(\varepsilon)}. \quad (3.4)$$

It is worth to mention that the topological derivative is defined by a limit passage when the small parameter governing the size of the topological perturbation goes to zero in (3.4). However, it can also be used as a steepest-descent direction in an optimization process like in any method based on the gradient of the cost functional.

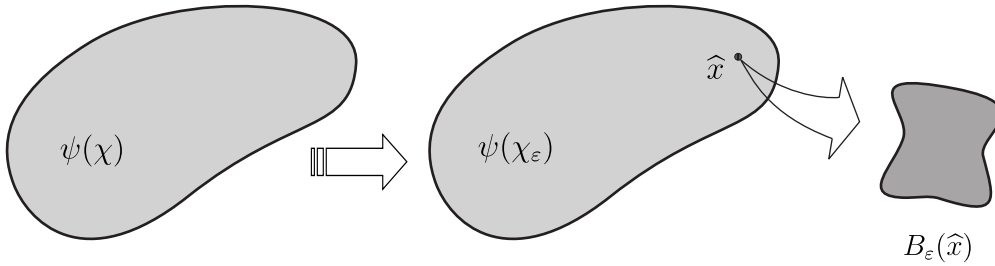


FIGURE 3. The topological derivative concept.

3.1. Perturbed problem. Now, let us introduce the topologically perturbed problem associated to the hydraulic fracture model. The idea consists in nucleating a circular inclusion, denoted by $B_\varepsilon(\hat{x})$, of radius ε and center at the arbitrary point $\hat{x} \in \Omega$, such that $\overline{B_\varepsilon(\hat{x})} \subset \Omega$. We assume that $B_\varepsilon(\hat{x})$ is submitted to a pressure load, which leads to a non-homogeneous transmission condition on the interface $\partial B_\varepsilon(\hat{x})$. See sketch in Figure 4. In this case $\chi_\varepsilon(\hat{x})$ is defined as follows:

$$\chi_\varepsilon(\hat{x}) = \mathbf{1}_\Omega - (1 - \gamma)\mathbf{1}_{B_\varepsilon(\hat{x})}, \quad (3.5)$$

where $\gamma = \gamma(x)$ is the contrast in the material properties. From these elements, we define a piecewise constant function of the form

$$\gamma_\varepsilon = \gamma_\varepsilon(x) := \begin{cases} 1 & \text{if } x \in \Omega \setminus \overline{B_\varepsilon}, \\ \gamma & \text{if } x \in B_\varepsilon. \end{cases} \quad (3.6)$$

The shape functional associated with the topologically perturbed problem is given by

$$\mathcal{F}_{\omega_\varepsilon}(u_\varepsilon) = \mathcal{J}_{\chi_\varepsilon}(u_\varepsilon) + \kappa|\omega_\varepsilon|, \quad (3.7)$$

where $\omega_\varepsilon = \omega \cup B_\varepsilon$ with $\omega \cap B_\varepsilon = \emptyset$. The total potential energy of the perturbed system, $\mathcal{J}_{\chi_\varepsilon}(u_\varepsilon)$, is given by

$$\mathcal{J}_{\chi_\varepsilon}(u_\varepsilon) = \frac{1}{2} \int_\Omega \sigma_\varepsilon(u_\varepsilon) \cdot \nabla u_\varepsilon^s dx - \int_\omega p_i \operatorname{div}(u_\varepsilon) dx - \int_{B_\varepsilon} p_i \operatorname{div}(u_\varepsilon) dx, \quad (3.8)$$

with the vector function u_ε solution of the following variational problem: Find $u_\varepsilon \in \mathcal{U}$, such that

$$\int_{\Omega} \sigma_\varepsilon(u_\varepsilon) \cdot \nabla \eta^s dx = \int_{\omega} p_i \operatorname{div}(\eta) dx + \int_{B_\varepsilon} p_i \operatorname{div}(\eta) dx, \quad \forall \eta \in \mathcal{V}, \quad (3.9)$$

where the Cauchy stress tensor $\sigma_\varepsilon(u_\varepsilon) = \gamma_\varepsilon \sigma(u_\varepsilon)$ with γ_ε given by (3.6).

The strong formulation associated with the variational problem (3.9) is given by: Find u_ε , such that:

$$\left\{ \begin{array}{ll} \operatorname{div} \sigma_\varepsilon(u_\varepsilon) = 0 & \text{in } \Omega, \\ \sigma_\varepsilon(u_\varepsilon) = \gamma_\varepsilon \sigma(u_\varepsilon), & \\ u_\varepsilon = 0 & \text{on } \partial\Omega, \\ \left. \begin{array}{l} \llbracket u_\varepsilon \rrbracket = 0 \\ \llbracket \sigma_\varepsilon(u_\varepsilon) \rrbracket n = -p_i n \end{array} \right\} & \text{on } \partial\omega, \\ \left. \begin{array}{l} \llbracket u_\varepsilon \rrbracket = 0 \\ \llbracket \sigma_\varepsilon(u_\varepsilon) \rrbracket n = -p_i n \end{array} \right\} & \text{on } \partial B_\varepsilon. \end{array} \right. \quad (3.10)$$

Again, the transmission conditions on the interfaces $\partial\omega$ and ∂B_ε stem from the variational formulation (3.9).

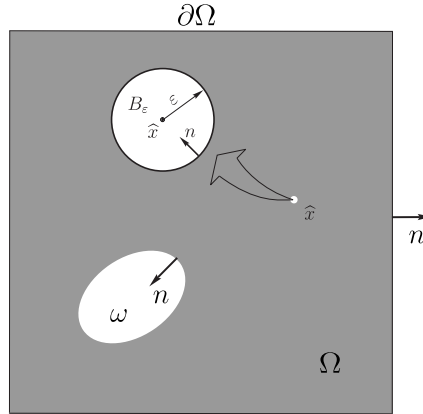


FIGURE 4. Perturbed problem.

3.2. Existence of the topological derivative. The existence of the associated topological derivative is ensured by the following result:

Lemma 3. *Let u_ε and u be solutions of problems (3.9) and (2.8), respectively. Then, the following estimate holds true:*

$$\|u_\varepsilon - u\|_{H^1(\Omega)} \leq C\varepsilon, \quad (3.11)$$

where C is a constant independent of the small parameter ε .

Proof. Let us subtract (2.8) from (3.9). Then, from the definition for the contrast (3.6), we obtain

$$\begin{aligned} \int_{B_\varepsilon} p_i \operatorname{div}(\eta) dx &= \int_{\Omega} (\sigma_\varepsilon(u_\varepsilon) - \sigma(u)) \cdot \nabla \eta^s dx \\ &= \int_{\Omega \setminus B_\varepsilon} (\sigma(u_\varepsilon) - \sigma(u)) \cdot \nabla \eta^s dx + \int_{B_\varepsilon} (\gamma \sigma(u_\varepsilon) - \sigma(u)) \cdot \nabla \eta^s dx. \end{aligned}$$

After adding and subtracting the term

$$\int_{B_\varepsilon} \gamma \sigma(u) \cdot \nabla \eta^s dx$$

in the above expression we have:

$$\int_{B_\varepsilon} p_i \operatorname{div}(\eta) dx = \int_{\Omega} \sigma_\varepsilon(u_\varepsilon - u) \cdot \nabla \eta^s dx + \int_{B_\varepsilon} (\gamma - 1) \sigma(u) \cdot \nabla \eta^s dx. \quad (3.12)$$

By taking $\eta = u_\varepsilon - u$ as test function in (3.12) we obtain the following equality:

$$\int_{\Omega} \sigma_\varepsilon(u_\varepsilon - u) \cdot \nabla (u_\varepsilon - u)^s dx = \int_{B_\varepsilon} (1 - \gamma) \sigma(u) \cdot \nabla (u_\varepsilon - u)^s dx + \int_{B_\varepsilon} p_i \operatorname{div}(u_\varepsilon - u) dx.$$

From the above expression, we have

$$\int_{\Omega} \sigma_\varepsilon(u_\varepsilon - u) \cdot \nabla (u_\varepsilon - u)^s dx = \int_{B_\varepsilon} \mathbb{T}(u) \cdot \nabla (u_\varepsilon - u)^s dx, \quad (3.13)$$

where we have introduced the notation

$$\mathbb{T}(u) = (1 - \gamma) \sigma(u) + p_i \mathbf{I}. \quad (3.14)$$

From Cauchy-Schwartz inequality it follows that

$$\begin{aligned} \int_{\Omega} \sigma_\varepsilon(u_\varepsilon - u) \cdot \nabla (u_\varepsilon - u)^s dx &\leq \|\mathbb{T}(u)\|_{L^2(B_\varepsilon)} \|\nabla (u_\varepsilon - u)\|_{L^2(B_\varepsilon)} \\ &\leq c_0 \varepsilon \|\nabla (u_\varepsilon - u)\|_{L^2(B_\varepsilon)} \\ &\leq c_1 \varepsilon \|u_\varepsilon - u\|_{H^1(\Omega)}. \end{aligned} \quad (3.15)$$

From the coercivity of the bilinear form on the left-hand side of (3.15) we have

$$c \|u_\varepsilon - u\|_{H^1(\Omega)}^2 \leq \int_{\Omega} \sigma_\varepsilon(u_\varepsilon - u) \cdot \nabla (u_\varepsilon - u)^s dx, \quad (3.16)$$

which leads to the result with $C = c_1/c$ independent of the small parameter ε . \square

3.3. Computation of the topological derivative. In order to evaluate the difference between the functionals $\mathcal{J}(u)$ and $\mathcal{J}_{\chi_\varepsilon}(u_\varepsilon)$, respectively defined in (2.7) and (3.8), we start by taking $\eta = u_\varepsilon - u$ as test function in the variational problem (2.8). Then we have the following equality

$$\int_{\Omega} \sigma(u) \cdot \nabla u^s dx = \int_{\Omega} \sigma(u) \cdot \nabla u_\varepsilon^s dx - \int_{\omega} p_i \operatorname{div}(u_\varepsilon - u) dx. \quad (3.17)$$

After replacing (3.17) into (2.7) we obtain

$$\mathcal{J}(u) = \frac{1}{2} \int_{\Omega} \sigma(u) \cdot \nabla u_\varepsilon^s dx - \frac{1}{2} \int_{\omega} p_i \operatorname{div}(u_\varepsilon + u) dx. \quad (3.18)$$

In the same way, let us set $\eta = u_\varepsilon - u$ as test function in the variational problem (3.9). Thus

$$\begin{aligned} \int_{\Omega} \sigma_\varepsilon(u_\varepsilon) \cdot \nabla u_\varepsilon^s dx &= \int_{\Omega} \sigma_\varepsilon(u_\varepsilon) \cdot \nabla u^s dx \\ &\quad + \int_{\omega} p_i \operatorname{div}(u_\varepsilon - u) dx + \int_{B_\varepsilon} p_i \operatorname{div}(u_\varepsilon - u) dx. \end{aligned} \quad (3.19)$$

After replacing (3.19) into (3.8), it follows

$$\mathcal{J}_{\chi_\varepsilon}(u_\varepsilon) = \frac{1}{2} \int_{\Omega} \sigma_\varepsilon(u_\varepsilon) \cdot \nabla u^s dx - \frac{1}{2} \int_{\omega} p_i \operatorname{div}(u_\varepsilon + u) dx - \frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(u_\varepsilon + u) dx. \quad (3.20)$$

From (3.18) and (3.20), the variation of the energy shape functionals can be written as

$$\begin{aligned} \mathcal{J}_{\chi_\varepsilon}(u_\varepsilon) - \mathcal{J}(u) &= \frac{1}{2} \int_{\Omega} \sigma_\varepsilon(u_\varepsilon) \cdot \nabla u^s dx - \frac{1}{2} \int_{\Omega} \sigma(u_\varepsilon) \cdot \nabla u^s dx \\ &\quad - \frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(u_\varepsilon + u) dx. \end{aligned} \quad (3.21)$$

Now, by taking into account the definition for the contrast γ_ε given by (3.6), we have

$$\begin{aligned} \mathcal{J}_{\chi_\varepsilon}(u_\varepsilon) - \mathcal{J}(u) &= \frac{1}{2} \int_{\Omega \setminus B_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla u^s dx + \frac{1}{2} \int_{B_\varepsilon} \gamma \sigma(u_\varepsilon) \cdot \nabla u^s dx \\ &\quad - \frac{1}{2} \int_{\Omega \setminus B_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla u^s dx - \frac{1}{2} \int_{B_\varepsilon} \sigma(u_\varepsilon) \cdot \nabla u^s dx - \frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(u_\varepsilon + u) dx. \end{aligned} \quad (3.22)$$

Let us add and subtract the term

$$\frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(u) dx. \quad (3.23)$$

Thus, the following expression is obtained after canceling the identical terms

$$\begin{aligned} \mathcal{J}_{\chi_\varepsilon}(u_\varepsilon) - \mathcal{J}(u) &= \int_{B_\varepsilon} \frac{\gamma - 1}{2\gamma} \sigma_\varepsilon(u_\varepsilon) \cdot \nabla u^s dx \\ &\quad - \int_{B_\varepsilon} p_i \operatorname{div}(u) dx - \frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(u_\varepsilon - u) dx. \end{aligned} \quad (3.24)$$

Note that the variation of the energy shape functional results in an integral concentrated into the inclusion B_ε . Therefore, in order to apply the definition for the topological derivative given by (3.2), we need to know the asymptotic behavior of the function u_ε with respect the small parameter ε . Thus, let us introduce the following ansatz:

$$u_\varepsilon = u + w_\varepsilon + \tilde{u}_\varepsilon, \quad (3.25)$$

where u is solution of the unperturbed problem (2.13), w_ε is solution to an auxiliary exterior problem and \tilde{u}_ε is the remainder.

After applying the operator σ_ε in the ansatz (3.25) we have

$$\sigma_\varepsilon(u_\varepsilon) = \sigma_\varepsilon(u) + \sigma_\varepsilon(w_\varepsilon) + \sigma_\varepsilon(\tilde{u}_\varepsilon). \quad (3.26)$$

By expanding $\sigma(u)$ in Taylor's series around the point \hat{x} we obtain

$$\sigma_\varepsilon(u_\varepsilon) = \sigma_\varepsilon(u)(\hat{x}) + \gamma_\varepsilon \nabla \sigma(u(\xi))(x - \hat{x}) + \sigma_\varepsilon(w_\varepsilon) + \sigma_\varepsilon(\tilde{u}_\varepsilon), \quad (3.27)$$

where ξ is an intermediate point between x and \hat{x} . On the boundary of the inclusion B_ε we have

$$\llbracket \sigma_\varepsilon(u_\varepsilon) \rrbracket n = -p_i n. \quad (3.28)$$

After evaluating (3.28) we obtain

$$(\sigma(u_\varepsilon)|_{\Omega \setminus \overline{B_\varepsilon}} - \gamma \sigma(u_\varepsilon)|_{B_\varepsilon}) n = -p_i n \quad \text{on} \quad \partial B_\varepsilon. \quad (3.29)$$

Then, let us evaluate (3.27) on ∂B_ε to have

$$-p_i n = (1 - \gamma) \sigma(u)(\hat{x}) n - \varepsilon (1 - \gamma) (\nabla \sigma(u(\xi)) n) n + \llbracket \sigma_\varepsilon(w_\varepsilon) \rrbracket n + \llbracket \sigma_\varepsilon(\tilde{u}_\varepsilon) \rrbracket n, \quad (3.30)$$

since $(x - \hat{x}) = -\varepsilon n$ on ∂B_ε . By choosing $\sigma_\varepsilon(w_\varepsilon)$ such as

$$\llbracket \sigma_\varepsilon(w_\varepsilon) \rrbracket n = ((\gamma - 1) \sigma(u)(\hat{x}) - p_i \mathbf{I}) n \quad \text{on} \quad \partial B_\varepsilon, \quad (3.31)$$

the following auxiliary boundary value problem is considered and formally obtained when $\varepsilon \rightarrow 0$: Find $\sigma_\varepsilon(w_\varepsilon)$ such that:

$$\begin{cases} \operatorname{div} \sigma_\varepsilon(w_\varepsilon) = 0 & \text{in } \mathbb{R}^2, \\ \sigma_\varepsilon(w_\varepsilon) \rightarrow 0 & \text{in } \infty, \\ \llbracket \sigma_\varepsilon(w_\varepsilon) \rrbracket n = \hat{u} & \text{on } \partial B_\varepsilon, \end{cases} \quad (3.32)$$

with $\hat{u} = ((\gamma - 1)\sigma(u)(\hat{x}) - p_i \mathbb{I})n$. The boundary value problem (3.32) admits an explicit solution. For $p_i = 0$, its solution can be found in [14, Ch. 5, pp. 156], for instance. Since the stress $\sigma_\varepsilon(w_\varepsilon)$ is uniform inside the inclusion, the solution of (3.32) for $p_i \neq 0$ can be written in a following compact form as

$$\sigma_\varepsilon(w_\varepsilon)|_{B_\varepsilon} = \mathbb{T}_\gamma \sigma(u)(\hat{x}) + \mathbb{T}_\gamma, \quad (3.33)$$

where \mathbb{T}_γ is a fourth order isotropic tensor given by

$$\mathbb{T}_\gamma = \frac{\gamma(1-\gamma)}{2(1+\beta\gamma)} \left(2\beta \mathbb{I} + \frac{\alpha-\beta}{1+\alpha\gamma} \mathbb{I} \otimes \mathbb{I} \right) \quad (3.34)$$

and \mathbb{T}_γ is a second order isotropic tensor written as

$$\mathbb{T}_\gamma = p_i \frac{\alpha\gamma}{1+\alpha\gamma} \mathbb{I}. \quad (3.35)$$

Remark 4. *The result shown in (3.33) fits the famous Eshelby problem. Formulated by Eshelby in 1957 [6] and 1959 [7], this problem plays a central role in the theory of elasticity involving the determination of effective elastic properties of materials with multiple inhomogeneities (inclusions, pores, defects, cracks, etc.). This important result represents one of the major advances in the continuum mechanics theory of the 20th century [11].*

Now we can construct $\sigma_\varepsilon(\tilde{u}_\varepsilon)$ in such a way that it compensates for the discrepancies introduced by the higher-order terms in ε as well as by the boundary-layer w_ε on the exterior boundary $\partial\Omega$. It means that the remainder \tilde{u}_ε must be solution to the following boundary value problem: Find \tilde{u}_ε such that:

$$\begin{cases} \operatorname{div} \sigma_\varepsilon(\tilde{u}_\varepsilon) = 0 & \text{in } \Omega, \\ \sigma_\varepsilon(\tilde{u}_\varepsilon) = \gamma_\varepsilon \sigma(\tilde{u}_\varepsilon), \\ \tilde{u}_\varepsilon = -w_\varepsilon & \text{on } \partial\Omega, \\ \llbracket \sigma_\varepsilon(\tilde{u}_\varepsilon) \rrbracket n = 0 & \text{on } \partial\omega, \\ \left. \begin{array}{l} \llbracket \tilde{u}_\varepsilon \rrbracket = 0 \\ \llbracket \sigma_\varepsilon(\tilde{u}_\varepsilon) \rrbracket n = \varepsilon h \end{array} \right\} & \text{on } \partial B_\varepsilon \end{cases} \quad (3.36)$$

with $h = (1-\gamma)(\nabla\sigma(u(\xi))n)n$. The estimate $\|\tilde{u}_\varepsilon\|_{H^1(\Omega)} = O(\varepsilon^2)$ for the remainder \tilde{u}_ε holds true. See, for instance, [14, Ch. 5, pp 155].

From the above results, we can evaluate the integrals in (3.24) explicitly. In fact, after replacing the ansatz for u_ε given by (3.25) in the first integral of (3.24) we have

$$\int_{B_\varepsilon} \sigma_\varepsilon(u_\varepsilon) \cdot \nabla u^s dx = \underbrace{\int_{B_\varepsilon} \sigma_\varepsilon(u) \cdot \nabla u^s dx}_{(a)} + \underbrace{\int_{B_\varepsilon} \sigma_\varepsilon(w_\varepsilon) \cdot \nabla u^s dx}_{(b)} + \mathcal{E}_1(\varepsilon). \quad (3.37)$$

The remainder $\mathcal{E}_1(\varepsilon)$ is given by

$$\begin{aligned} \mathcal{E}_1(\varepsilon) &= \int_{B_\varepsilon} \sigma_\varepsilon(\tilde{u}_\varepsilon) \cdot \nabla u^s dx \\ &\leq \|\sigma_\varepsilon(\tilde{u}_\varepsilon)\|_{L^2(B_\varepsilon)} \|\nabla u\|_{L^2(B_\varepsilon)} \\ &\leq c_1 \|\tilde{u}_\varepsilon\|_{H^1(\Omega)} \|\nabla u\|_{L^2(B_\varepsilon)} \leq c_2 \varepsilon^3 = O(\varepsilon^3), \end{aligned} \quad (3.38)$$

where we have used the Cauchy-Schwarz inequality together with the estimation for the remainder \tilde{u}_ε . The term (a) in (3.37) can be developed in power of ε as follows

$$\begin{aligned} \int_{B_\varepsilon} \sigma_\varepsilon(u) \cdot \nabla u^s dx &= \int_{B_\varepsilon} \gamma \sigma(u) \cdot \nabla u^s dx \\ &= \pi \varepsilon^2 \gamma \sigma(u)(\hat{x}) \cdot \nabla u^s(\hat{x}) + \mathcal{E}_2(\varepsilon), \end{aligned} \quad (3.39)$$

with the remainder $\mathcal{E}_2(\varepsilon)$ defined as

$$\begin{aligned} \mathcal{E}_2(\varepsilon) &= \int_{B_\varepsilon} (h(x) - h(\hat{x})) dx \\ &\leq \|h(x) - h(\hat{x})\|_{L^2(B_\varepsilon)} \|1\|_{L^2(B_\varepsilon)} \\ &\leq c_1 \varepsilon \|x - \hat{x}\|_{L^2(B_\varepsilon)} \leq c_2 \varepsilon^3 = O(\varepsilon^3), \end{aligned} \quad (3.40)$$

where we have introduced the notation

$$h(x) - h(\hat{x}) = \sigma(u)(x) \cdot \nabla u^s(x) - \sigma(u)(\hat{x}) \cdot \nabla u^s(\hat{x}). \quad (3.41)$$

Note that, we have used again the Cauchy-Schwarz inequality and the interior elliptic regularity of function u . Since the exact solution of the auxiliary problem (3.32) is known, the term (b) in (3.37) can be written as

$$\int_{B_\varepsilon} \sigma_\varepsilon(w_\varepsilon) \cdot \nabla u^s dx = \pi \varepsilon^2 \nabla u^s(\hat{x}) \cdot (\mathbb{T}_\gamma \sigma(u)(\hat{x}) + \mathbb{T}_\gamma) + \mathcal{E}_3(\varepsilon). \quad (3.42)$$

The remainder $\mathcal{E}_3(\varepsilon)$ is given by

$$\begin{aligned} \mathcal{E}_3(\varepsilon) &= \int_{B_\varepsilon} \sigma_\varepsilon(w_\varepsilon) \cdot (\nabla u^s - \nabla u^s(\hat{x})) dx \\ &\leq \|\sigma_\varepsilon(w_\varepsilon)\|_{L^2(B_\varepsilon)} \|\nabla u - \nabla u(\hat{x})\|_{L^2(B_\varepsilon)} \\ &\leq c_1 \varepsilon \|x - \hat{x}\|_{L^2(B_\varepsilon)} \leq c_2 \varepsilon^3 = O(\varepsilon^3), \end{aligned} \quad (3.43)$$

where we have used again the Cauchy-Schwarz inequality and the interior elliptic regularity of function u .

The second term in (3.24) can be developed as follows

$$\int_{B_\varepsilon} p_i \operatorname{div}(u) dx = \pi \varepsilon^2 p_i \operatorname{div}(u)(\hat{x}) + \mathcal{E}_4(\varepsilon), \quad (3.44)$$

where the remainder $\mathcal{E}_4(\varepsilon)$ is defined as

$$\begin{aligned} \mathcal{E}_4(\varepsilon) &= \int_{B_\varepsilon} p_i (\operatorname{div}(u) - \operatorname{div}(u)(\hat{x})) dx \\ &\leq c_1 \|x - \hat{x}\|_{L^2(B_\varepsilon)} \|1\|_{L^2(B_\varepsilon)} \leq c_2 \varepsilon^3 = O(\varepsilon^3). \end{aligned} \quad (3.45)$$

Once again, we have used the Cauchy-Schwarz inequality together with the interior elliptic regularity of function u .

After replacing the ansatz for u_ε given by (3.25) into the last term of (3.24) we have

$$\frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(u_\varepsilon - u) dx = \frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(w_\varepsilon + \tilde{u}_\varepsilon) dx = \frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(w_\varepsilon) dx + \mathcal{E}_5(\varepsilon). \quad (3.46)$$

where the remainder $\mathcal{E}_5(\varepsilon)$ has the following bound thanks to the estimate for \tilde{u}_ε

$$\begin{aligned} \mathcal{E}_5(\varepsilon) &= \frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(\tilde{u}_\varepsilon) dx \\ &\leq c_1 \|\nabla \tilde{u}_\varepsilon\|_{L^2(B_\varepsilon)} \|1\|_{L^2(B_\varepsilon)} \\ &\leq c_2 \varepsilon \|\tilde{u}_\varepsilon\|_{H^1(\Omega)} \leq c_2 \varepsilon^3 = O(\varepsilon^3). \end{aligned} \quad (3.47)$$

By using the constitutive relation and after algebraic manipulations, we have

$$\frac{1}{2} \int_{B_\varepsilon} p_i \operatorname{div}(w_\varepsilon) dx = \frac{1}{2} \int_{B_\varepsilon} \frac{p_i}{2\gamma\rho(\mu + \lambda)} \operatorname{tr}\sigma_\varepsilon(w_\varepsilon) dx, \quad (3.48)$$

where $\operatorname{tr}\sigma_\varepsilon(w_\varepsilon)$, evaluated inside the inclusion, is given by

$$\operatorname{tr}\sigma_\varepsilon(w_\varepsilon)|_{B_\varepsilon(\hat{x})} = \frac{\alpha\gamma}{1 + \alpha\gamma} ((1 - \gamma)\operatorname{tr}\sigma(u)(\hat{x}) + 2p_i). \quad (3.49)$$

From the above results, the variation of the energy shape functionals, given by (3.24), can be developed in power of ε as follows

$$\begin{aligned} \mathcal{J}_{\chi_\varepsilon}(u_\varepsilon) - \mathcal{J}(u) &= -\pi\varepsilon^2 \frac{1-\gamma}{2\gamma} [\gamma\sigma(u)(\hat{x}) + (\mathbb{T}_\gamma\sigma(u)(\hat{x}) + \mathbb{T}_\gamma)] \cdot \nabla u^s(\hat{x}) \\ &\quad - \pi\varepsilon^2 p_i \operatorname{div}(u)(\hat{x}) - \pi\varepsilon^2 \frac{\alpha}{2} \frac{1-\gamma}{1+\alpha\gamma} p_i \operatorname{div}(u)(\hat{x}) \\ &\quad - \pi\varepsilon^2 \frac{p_i^2}{2\mu\rho(1+\alpha\gamma)} + \sum_{i=1}^5 \mathcal{E}_i(\varepsilon), \end{aligned} \quad (3.50)$$

where the remainders $\mathcal{E}_i(\varepsilon) = o(\varepsilon^2)$, for $i = 1, \dots, 5$, as previously shown. By defining the function $f(\varepsilon) = \pi\varepsilon^2$ and after applying the topological derivative concept in (3.50), we obtain

$$D_T \mathcal{J}(\hat{x}) = -\mathbb{P}_\gamma \sigma(u)(\hat{x}) \cdot \nabla u^s(\hat{x}) - \frac{1+\alpha}{1+\alpha\gamma} p_i \operatorname{div}(u)(\hat{x}) - \frac{1}{2\rho\mu} \frac{p_i^2}{(1+\alpha\gamma)}, \quad (3.51)$$

where \mathbb{P}_γ is a fourth order isotropic tensor given by

$$\mathbb{P}_\gamma = \frac{1}{2} \frac{1-\gamma}{1+\beta\gamma} \left((1+\beta)\mathbb{I} + \frac{1}{2}(\alpha-\beta) \frac{1-\gamma}{1+\alpha\gamma} \mathbb{I} \otimes \mathbb{I} \right), \quad (3.52)$$

with the coefficients α and β defined as

$$\alpha = \frac{\lambda + \mu}{\mu} \quad \text{and} \quad \beta = \frac{\lambda + 3\mu}{\lambda + \mu}. \quad (3.53)$$

For more details concerning the polarization tensor (3.52), see for instance [3].

Finally, the topological derivative of the shape functional (2.6) with respect to the nucleation of a small circular pressurized inclusion is given by the sum

$$D_T \mathcal{F}_\omega(x) = D_T \mathcal{J}(x) + \kappa D_T |\omega| \quad \forall x \in \Omega, \quad (3.54)$$

where $D_T \mathcal{J}(x)$ is given by (3.51) while the topological derivative of the Griffith-type dissipation energy term, $\kappa D_T |\omega|$, is trivially obtained and given by

$$\kappa D_T |\omega|(x) = \begin{cases} +\kappa, & \text{if } x \in \Omega \setminus \bar{\omega}, \\ -\kappa, & \text{if } x \in \omega. \end{cases} \quad (3.55)$$

3.4. Expression of the topological derivative. Since we are using a very weak material to replace the pressurized region, we can take the limit cases $\gamma \rightarrow 0$ and $\gamma \rightarrow \infty$ in (3.54). Formally, for $\gamma \rightarrow 0$ the inclusion represents a hole and the transmission condition on the boundary of the inclusion degenerates itself to non-homogeneous Neumann boundary condition. In this case the topological derivative evaluated within the elastic material $\Omega \setminus \bar{\omega}$ becomes

$$D_T \mathcal{F}_\omega(x) = -\mathbb{P}_0 \sigma(u)(x) \cdot \nabla u^s(x) - (1 + \alpha) p_i \operatorname{div}(u)(x) - \frac{p_i^2}{2\mu} + \kappa, \quad \forall x \in \Omega, \quad (3.56)$$

with the polarization tensor \mathbb{P}_0 given by

$$\mathbb{P}_0 = \frac{1 + \beta}{2} \mathbb{I} + \frac{\alpha - \beta}{4} \mathbf{I} \otimes \mathbf{I}. \quad (3.57)$$

In addition, for $\gamma \rightarrow \infty$, the elastic inclusion leads to a rigid inclusion. In this case the topological derivative evaluated into the compliant material ω results in

$$D_T \mathcal{F}_\omega(x) = -\mathbb{P}_\infty \sigma(u)(x) \cdot \nabla u^s(x) - \kappa, \quad \forall x \in \omega, \quad (3.58)$$

where the polarization tensor \mathbb{P}_∞ is given by

$$\mathbb{P}_\infty = -\frac{1 + \beta}{2\beta} \mathbb{I} + \frac{\alpha - \beta}{4\alpha\beta} \mathbf{I} \otimes \mathbf{I}. \quad (3.59)$$

Remark 5. *The same formula (3.54) holds true for heterogeneous medium [9], provided that the heterogeneity is locally Lipschitz continuous.*

4. TOPOLOGY OPTIMIZATION ALGORITHM

In this section the obtained topological derivative expression is used to devise a simple topology optimization algorithm specifically designed to simulate the whole nucleation and propagation process of hydraulic fracturing. This algorithm was originally proposed in [18]. It is based on the fact that the introduction of infinitesimal inclusion at the region where the topological derivative is negative allow for a decreasing on the values of the shape functional. For the sake of completeness, the adapted version of the algorithm to the context of hydraulic fracturing process is presented below. For more details see [18].

The present algorithm is based on the introduction of an inclusion at the region where the topological derivative is negative. If the size of the inclusion is small enough to corroborate with the theory, but at the same time large enough to be treated numerically, it is expected that the shape functional (2.6) decreases. The size of inclusion is associated with the region ω^* where the topological derivative field is negative, i.e.,

$$\omega^* := \{x \in \Omega : D_T \mathcal{F}_\omega(x) < 0\} . \quad (4.1)$$

In principle ω^* must not be a connected subset, that is, there might be nucleation of damage in front of the previously damage zone, but also elsewhere in the body. In the first case, nucleation of damage yields evolution of the damage set, whereas in the latter it means genuine damage nucleation. Let us emphasize that from a theoretical point of view, the topological derivative holds away from the damage region and for an infinitesimal inclusion only. On the other hand, the topological derivative can be used as a steepest-descent direction in the optimization process like in any method based on the gradient of the objective functional. Therefore, for practical purposes, since the numerical method introduces a grid of finite size, we will consider nucleation of inclusions of finite sizes but small enough such that a decreasing of the proposed functional in each iteration is ensured.

The algorithm can be designed either by nucleating only at those points where the topological derivative achieves its minimum, or at all points where it is negative. On the other hand, an intermediate choice would be to calibrate the size of the inclusion to be nucleated according to the characteristic size of the previously damaged region. This choice will be provided by the model parameter $\beta \in (0, 1)$, with the extreme choices given by $\beta = 0$ (minimum points only), and $\beta = 1$ (the whole negative region), respectively. To this aim, let us introduce the quantity

$$D_T \mathcal{F}_\omega^* := \min_{x \in \omega^*} D_T \mathcal{F}_\omega(x) , \quad (4.2)$$

which allows us to define the inclusion to be nucleated $\omega^\beta \subset \omega^*$ as follows

$$\omega^\beta := \{x \in \omega^* : D_T \mathcal{F}_\omega(x) \leq (1 - \beta) D_T \mathcal{F}_{\omega^*}\} , \quad (4.3)$$

where $\beta \in (0, 1)$ is chosen such that $|\omega^\beta| \approx (\pi l^2)/4$ (with $l \leq \delta$), so that the size of the inclusion to be nucleated is here related to the width δ of the initial damage. Therefore, if the initial damage is crack-like (δ small), β will be taken as small as to satisfy $|\omega^\beta| \leq (\pi l^2)/4$. By this choice, a damage will evolve like a crack. As a matter of fact, the parameter β induces a threshold for the topological derivative $D_T \mathcal{F}_\omega(x)$ and the volume of the inclusion will only depend on l , while its shape and location will depend on the contour lines (level-sets) of $D_T \mathcal{F}_\omega$. We will show through some numerical experiments that this strategy ensures a decreasing of the proposed functional at each iteration, provided that the size of the inclusion to be nucleated ω^β is small enough.

The algorithm can be outlined as follows. Given the solution of the linear elasticity system (2.8), the associated topological derivative field (3.54) is evaluated. If the field is positive everywhere or $|\omega^*| < (\pi l^2)/4$, a perturbation of size $(\pi l^2)/4$ at any point of the domain is likely to increase the value of the functional. In this case, the algorithm will not propagate the damage, and it is possible to increase the pressure p_i further and run a new analysis. On the contrary, if the topological derivative field is negative in some undamaged region and the condition $|\omega^*| \geq (\pi l^2)/4$ is fulfilled, a damage ω^β will be nucleated inside ω^* , with $\beta : |\omega^\beta| \approx (\pi l^2)/4$. Schematically, one can see the newly-damaged region as an half-disk of radius $l/2$ located at the tip of the pre-existing damage. Since the nucleation of a new damage ω^β modifies the problem, the solution to the elasticity system associated with the new topology need to be computed again. Finally, the new topological derivative field is evaluated and the process is repeated until the condition $|\omega^*| \geq (\pi l^2)/4$ is no more fulfilled for any pressure increment. The elasticity system is solved by the finite element method. In order to improve the numerical results, the mesh at the crack tip is intensified in each iteration of the optimization process. The above procedure written in the form of pseudo-code is given in Algorithm 1.

Algorithm 1: The damage evolution algorithm.

input : $\Omega, \omega, l, N, p_0, \Delta p_i$
output: The optimal topology ω^*

- 1 **for** $i = 1 : N$ **do**
- 2 solve elasticity system (2.8);
- 3 evaluate the topological derivative $D_T \mathcal{F}_\omega$ according to (3.54);
- 4 compute the threshold ω^* from (4.1);
- 5 **while** $|\omega^*| \geq (\pi l^2)/4$ **do**
- 6 intensify the mesh at the crack tip;
- 7 solve elasticity system and evaluate $D_T \mathcal{F}_\omega$;
- 8 compute the threshold ω^* from (4.1);
- 9 compute the threshold ω^β from (4.3);
- 10 nucleated new inclusion ω^β inside ω^* ;
- 11 update the damaged region: $\omega \leftarrow \omega \cup \omega^\beta$;
- 12 solve elasticity system and evaluate $D_T \mathcal{F}_\omega$;
- 13 compute the threshold ω^* from (4.1);
- 14 **end while**
- 15 **end for**

5. NUMERICAL EXPERIMENTS

As mentioned in Section 1, the reference domain Ω stands for one block of the reservoir, i.e., a limited region which contains an initial damage representing a single geological fault, see Figure 1. The topology is identified by the elastic material distribution and the compliant material is used to represent the geological fault. We assume that in all examples the structure is under plane strain assumption and that the total intensity of the pressure p was divided into N uniform increments. In addition, the elasticity problem is discretized by using linear triangular elements only.

5.1. Elementary example. In this first example, the hold-all domain Ω is given by a square with dimension $(5 \times 5)m^2$ as shown in Figure 5. Homogeneous Dirichlet boundary conditions are considered in all sides of the domain. A pre-existing geological fault, represented by the initial damage of length h and width δ , is located at the center of the bottom side immediately above the pressurization well. The material properties such as the modulus of elasticity E and the Poisson ratio ν correspond to the values used in [15]. In addition, the inclusion is made of a material with an elasticity modulus $\rho_0 E$ and its diameter is specified by the parameter l . The total intensity of the pressure is $p = 8$ MPa and was divided into $N = 200$ uniform increments. All these data are summarized in Table 1.

TABLE 1. Elementary example: Parameters.

Parameter	Value	Parameter	Value
h	1,0 m	E	30 GPa
δ	0,025 m	ρ_0	10^{-6}
l	$(2/3)\delta$	ν	0,3
p	8 MPa	κ_s	320,0 J/m

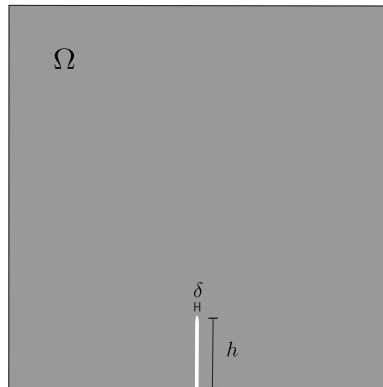


FIGURE 5. Elementary example: Geometry.

5.1.1. Critical pressure. As mentioned in Section 2, it is necessary to verify whether the proposed hydraulic fracture model permits the characterization of the fault-activation pressure. To this aim, five tests were made with different values for the initial width δ of the damage, namely $\delta \in \{\frac{1}{20}, \frac{1}{40}, \frac{1}{80}, \frac{1}{160}, \frac{1}{320}\}$ [m]. The parameters were maintained according to Table 1. The critical pressure p_c was selected as the value of the current pressure which allows the nucleation of the first inclusion, that is, when the condition $|\omega^*| \geq (\pi l^2)/4$ holds for the first time. Figure 6 illustrates the critical pressure obtained

for the different tests, which are normalized according to the first estimate found for the critical pressure p_c^0 . Therefore, the introduction of the parameter κ_δ through (2.15) allows for dealing with a feasible critical pressure as shown in Figure 6 (blue bullet line). We claim however that it is an *ad hoc* correction of the model which works for $\delta > 0$. The limiting case $\delta \rightarrow 0$ is much more involved and has been partially addressed in [17], for instance. However, the proper variational limit is currently out of reach for the planar vectorial problem (i.e., without the anti-plane assumption). As expected, with the

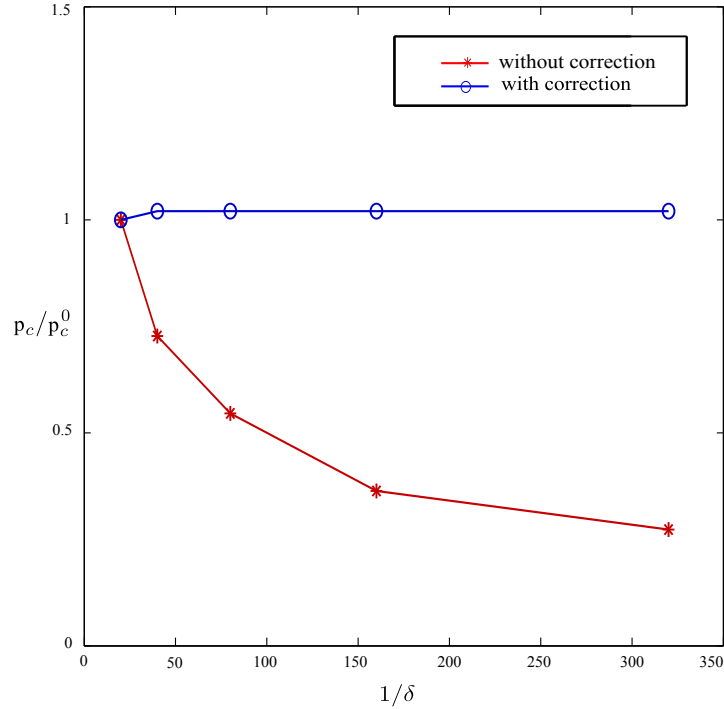


FIGURE 6. Elementary example: Convergence analysis for the critical pressure.

decrease of the width δ , the energy density at the crack tip increases. Note that without a scale factor correction, the critical pressure decreases towards zero. On the other hand, the use of the factor δ leads to an asymptotic behavior for the critical pressure.

Remark 6. *The result shown in Figure 6 can be seen as a numerical evidence of the mathematical convergence of the proposed approach to a hydraulic fracture model in its strict sense. Therefore, the study of such underlying mathematical convergence is an important topic which will be treated in future works.*

5.1.2. *Damage evolution.* The final result obtained at iteration number 215 is shown in Figure 7, after which the program was interrupted. Note that the crack trajectory occurs in a straight line as expected. The pressure has been incremented 80 times to comply with the propagation criterion. Moreover, the observed critical pressure is $p_c = 3.2$ MPa. Note that the model dissipates energy at each iterations, as shown in Figure 8.

5.2. **Transverse wells.** This second example has the same geometry and boundary conditions of the previous one. However, in the present case two transverse wells centered at the points $c_1 = (2.8, 1.5)$ and $c_2 = (2.8, 2.5)$ and with diameters $d_1 = 0.3$ m and $d_2 = 0.7$ m, respectively, are considered. See Figures 9(a) and 10(a). In this example, the total intensity of the pressure is $p = 6$ MPa and was divided into $N = 150$ uniform increments. The remainder parameters being chosen according to Table 1. In addition, two different situations are considered. The first one (case 1) considers that the transverse

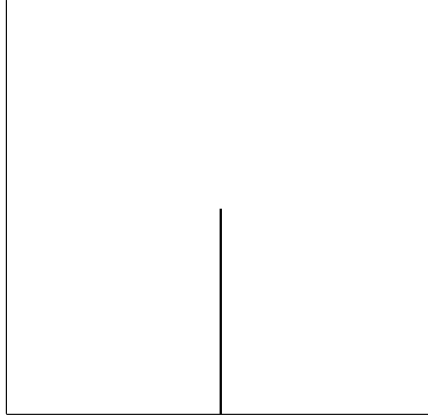
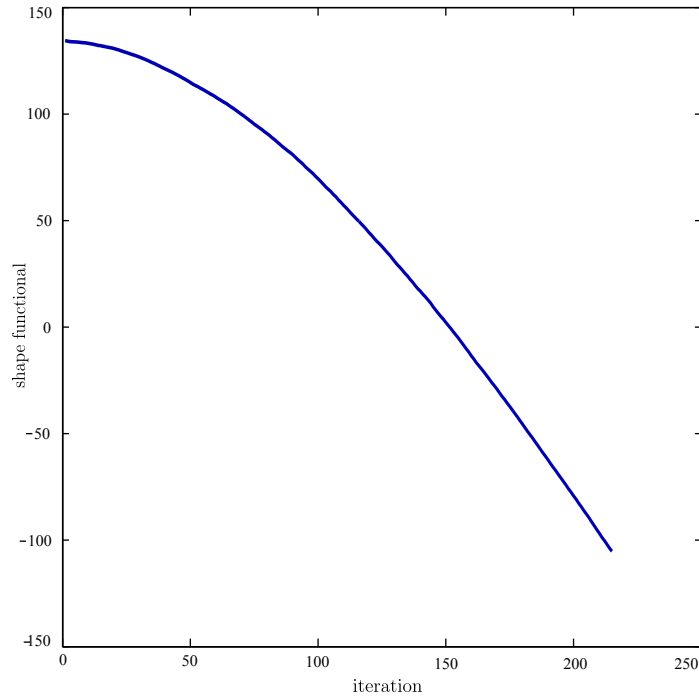


FIGURE 7. Elementary example: Final result.

FIGURE 8. Elementary example: Total energy $\mathcal{F}_\omega(u)$ from (2.6).

wells are not pressurized. In the second situation (case 2) the transverse wells are pressurized and the intensity of the pressure is the same as that inside the initial damage. Thus, the scope of this study is the influence of these transverse wells on the crack trajectory.

The final results are shown in Figures 9(b) and 10(b). In the case 1 the observed critical pressure is $p_c = 3.24$ MPa. Note that in this case the smaller *no-pressurized* transverse well only affect the crack trajectory. After then, the crack tip attains the second transverse well. In the case 2, the observed critical pressure is $p_c = 3.2$ MPa. In this case, the smaller *pressurized* transverse well attracts abruptly the crack trajectory. After then, the crack tip attains the second transverse well again. This fact suggests a potential strategy to control the crack trajectories by inserting transverse wells into the reservoir. In addition, it can be verified from the case 2 that the proposed algorithm was able to activate the mechanism of damage nucleation, independently of any initial

damaged region on the boundary of the smaller transverse well. As matter of fact, the critical pressure associated to the nucleation phenomenon was $p_c = 4.08$ MPa. Finally, the behavior of the square root of the strain energy, defined by

$$\mathcal{E}(u) = \sqrt{\frac{1}{2} \int_{\Omega} \sigma(u) \cdot \nabla u^s}, \quad (5.1)$$

in both cases, is shown in Figure 11.

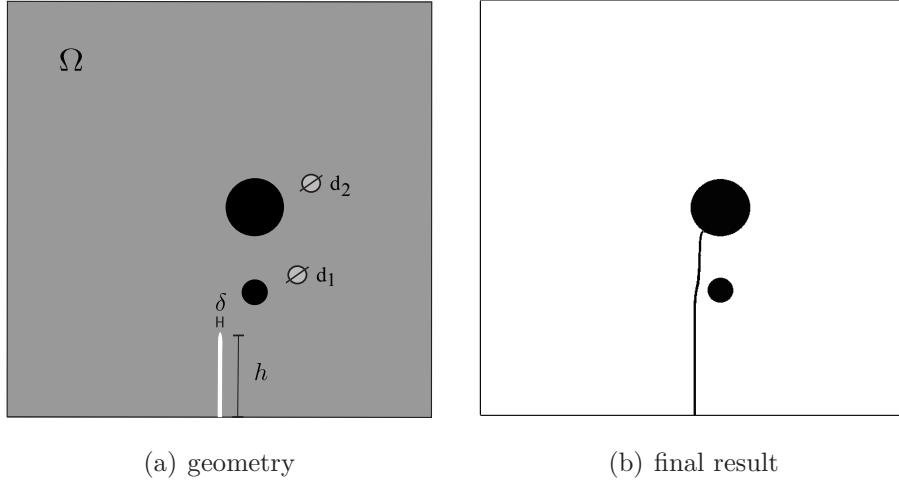


FIGURE 9. Case 1: No-pressurized transverse wells.

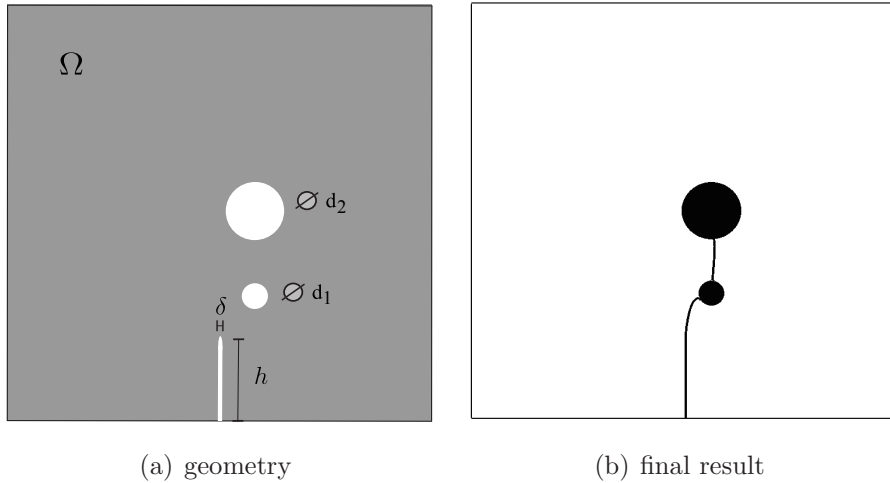


FIGURE 10. Case 2: Pressurized transverse wells.

5.3. Stratified block. In this example, we consider an heterogeneous material: the block is composed by two layers with different elasticity modulus, namely, $E_1 = 30$ GPa and $E_2 = 60$ GPa. In addition, the geometry and boundary conditions are the same as proposed in the elementary example of Section 5.1. The different cases treated in this example differ from each other by the spatial distribution of the material properties E_1 and E_2 , as shown in Figures 12(a) and 13(a). The remainder parameters being chosen according to Table 1.

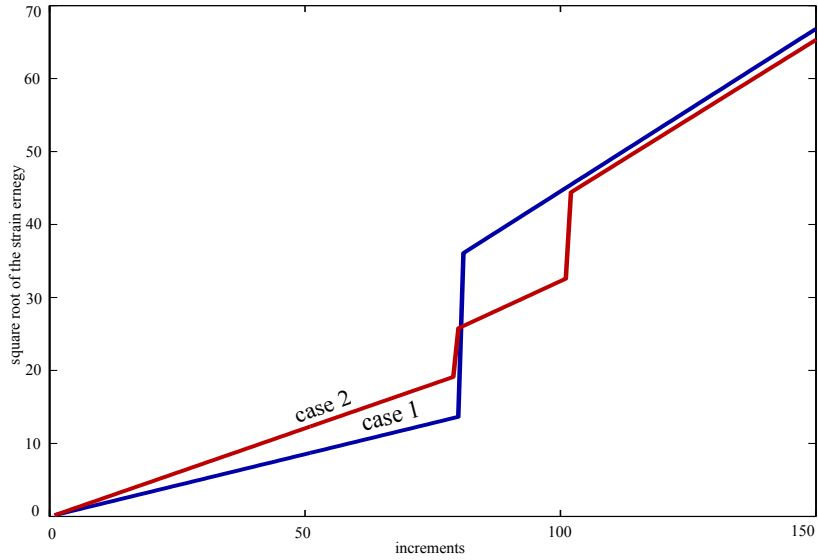


FIGURE 11. Transverse wells: Square root of the strain energy $\mathcal{E}(u)$ from (5.1).

The final results are shown in Figures 12(b) and 13(b). In the first case, the observed critical pressure is $p_c = 3.32$ MPa. Note that in this scenario, the trajectory of the fracture follows the direction of the interface between the two materials when the crack tip attains the stiffer layer. In the second case, the observed critical pressure is $p_c = 4.4$ MPa. In this situation the trajectory of the fracture only suffers a little change in its direction when the crack tip attains the weaker layer.

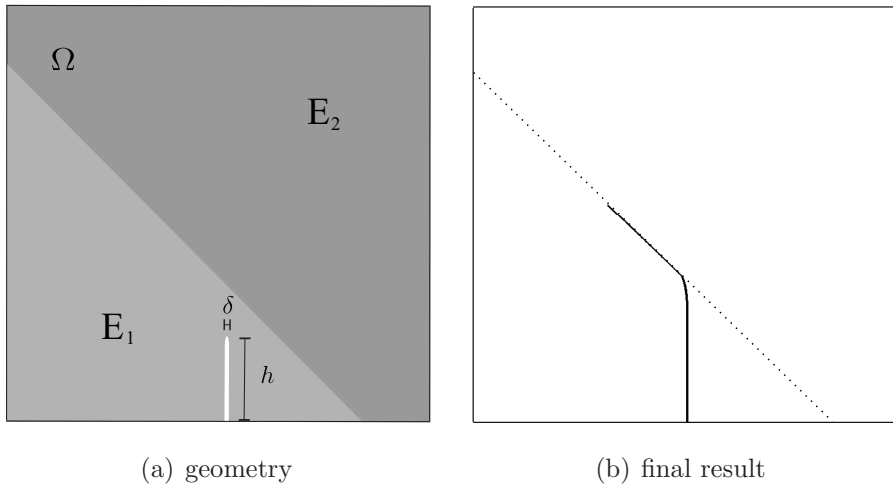


FIGURE 12. Stratified block: Case 1.

5.4. Heterogeneous medium. In this last example a heterogeneous medium is considered. The geometry, boundary conditions and the parameters are the same of the elementary example of Section 5.1. However, in this case the Young modulus E is corrupted with White Gaussian Noise (WGN) of zero mean and standard deviation η . Therefore, E is replaced by $E_\eta = E(1 + s\eta)$, where $s : \Omega \rightarrow \mathbb{R}$ is a function assuming random values in the interval $(0, 1)$ and $\eta = 5$ corresponds to the noise level. The Figures 14(a) and 14(b) shows the corrupted Young modulus $E_\eta(x)$ and the final result, respectively. The observed critical pressure is $p = 7.92$ MPa. Note that, due to the medium heterogeneity,

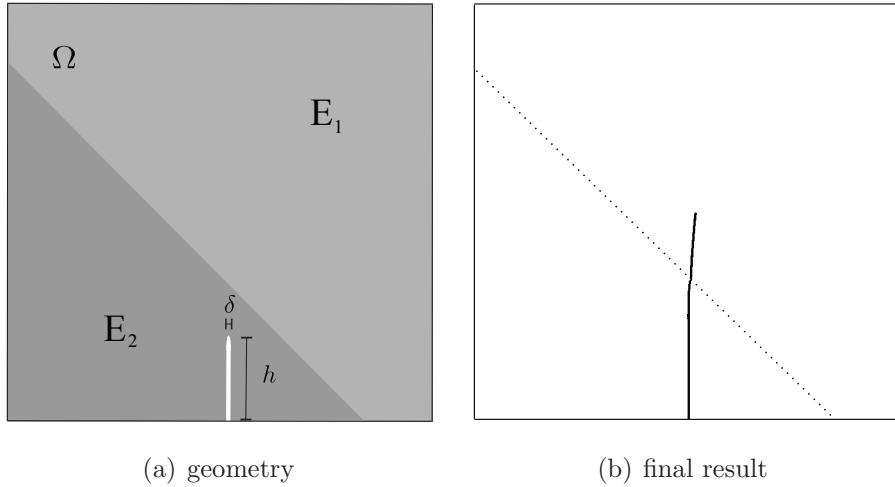


FIGURE 13. Stratified block: Case 2.

we can observe kinking and bifurcations phenomena, which is in agreement with what it is expected from the physical point of view.

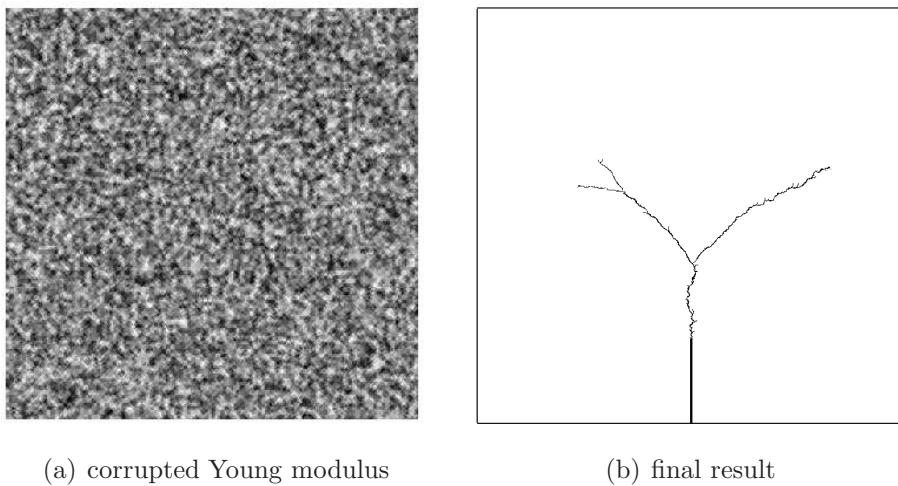


FIGURE 14. Heterogeneous medium.

6. CONCLUDING REMARKS

This paper has demonstrated that the linear and variational fracture model introduced by Francfort and Marigo may be applied to hydraulic fracturing process, by means of an original use of topological derivative concept. In particular, a novel hydraulic fracture model obtained by adapting the one introduced by Francfort and Marigo to the context of hydraulic fracturing process has been proposed. A shape functional given by the sum of the total potential energy of the system with a Griffith-type dissipation energy term has been minimized with respect to a set of ball-shaped pressurized inclusions by using the topological derivative concept. It means that, the topological asymptotic expansion of such shape functional with respect to the nucleation of a circular inclusion endowed with non-homogeneous transmission condition on its boundary, has been rigorously developed. In addition, we have shown that the associated topological derivative corroborates with the famous Eshelby theorem. The obtained result has been used to

devise a topology optimization algorithm specifically designed to simulate the whole nucleation and propagation process of hydraulic fracturing. The strikingly simplicity of the proposed topological derivative-based fracture modelling should be noted. In fact, since the loading, given by the prescribed pressure acting within the damage region, comes out naturally from the variational formulation, just a minimal number of user-defined algorithmic parameters is required. Finally, we have provided four test cases which showed the potential of our approach. From this test cases, typical features of hydraulic fracturing process, including the characterization of the fault-activation pressure and specific crack path growth, allowing for kinking and bifurcations has been observed. Further study is related to the underlying mathematical convergence, and the three-dimensional case.

ACKNOWLEDGEMENTS

This research was partly supported by CNPq (Brazilian Research Council), CAPES (Brazilian Higher Education Staff Training Agency), ANP (National Agency of Petroleum, Natural Gas and Biofuels) and FAPERJ (Research Foundation of the State of Rio de Janeiro). These supports are gratefully acknowledged. Second author was supported by the FCT Starting Grant “Mathematical theory of dislocations: geometry, analysis, and modelling” (IF/00734/2013).

REFERENCES

- [1] G. Allaire, F. Jouve, and N. Van Goethem. Damage and fracture evolution in brittle materials by shape optimization methods. *Journal of Computational Physics*, 230(12):5010–5044, 2011.
- [2] L. Ambrosio and V. Tortorelli. On the approximation of free discontinuity problems. *Bollettino dell’Unione Matematica Italiana*, 6:105–123, 1992.
- [3] H. Ammari and H. Kang. *Polarization and moment tensors with applications to inverse problems and effective medium theory*. Applied Mathematical Sciences vol. 162. Springer-Verlag, New York, 2007.
- [4] B. Bourdin, G. A. Francfort, and J. J. Marigo. Numerical experiments in revisited brittle fracture. *Journal of the Mechanics and Physics of Solids*, 48(4):797–826, 2000.
- [5] B. Bourdin, G. A. Francfort, and J. J. Marigo. The variational approach to fracture. *Journal of Elasticity*, 91(1-3):5–148, 2008.
- [6] J. D. Eshelby. The determination of the elastic field of an ellipsoidal inclusion, and related problems. *Proceedings of the Royal Society: Section A*, 241:376–396, 1957.
- [7] J. D. Eshelby. The elastic field outside an ellipsoidal inclusion, and related problems. *Proceedings of the Royal Society: Section A*, 252:561–569, 1959.
- [8] G. A. Francfort and J. J. Marigo. Stable damage evolution in a brittle continuous medium. *European Journal of Mechanics, A/Solids*, 12(2):149–189, 1993.
- [9] S. M. Giusti, A. Ferrer, and J. Oliver. Topological sensitivity analysis in heterogeneous anisotropic elasticity problem. theoretical and computational aspects. *Computer Methods in Applied Mechanics and Engineering*, 311:134–150, 2016.
- [10] G. Hattori, Jon Trevelyan, C. E. Augarde, W. M. Coombs, and A. C. Aplin. Numerical simulation of fracking in shale rocks: Current state and future approaches. *Archives of Computational Methods in Engineering*, 24(2):281–317, 2017.
- [11] M. Kachanov, B. Shafiro, and I. Tsukrov. *Handbook of Elasticity Solutions*. Kluwer Academic Publishers, Dordrecht, 2003.
- [12] A. Karma, D. A. Kessler, and H. Levine. Phase-field model of mode III dynamic fracture. *Physical Review Letters*, 87(4):045501, 2001.
- [13] G. Dal Maso and F. Iurlano. Fracture models as Gamma-limits of damage models. *Communications on Pure and Applied Mathematics*, 12(4):1657–1686, 2013.
- [14] A. A. Novotny and J. Sokolowski. *Topological derivatives in shape optimization*. Interaction of Mechanics and Mathematics. Springer-Verlag, Berlin, Heidelberg, 2013.
- [15] L. C. Pereira, L. J. N. Guimarães, B. Horowitz, and M. Sánchez. Coupled hydro-mechanical fault reactivation analysis incorporating evidence theory for uncertainty quantification. *Computers and Geotechnics*, 56:202–215, 2014.

- [16] J. Sokółowski and A. Żochowski. On the topological derivative in shape optimization. *SIAM Journal on Control and Optimization*, 37(4):1251–1272, 1999.
- [17] N. Van Goethem and A. A. Novotny. Crack nucleation sensitivity analysis. *Mathematical Methods in the Applied Sciences*, 33(16):1978–1994, 2010.
- [18] M. Xavier, E. A. Fancello, J. M. C. Farias, N. Van Goethem, and A. A. Novotny. Topological derivative-based fracture modelling in brittle materials: A phenomenological approach. *Engineering Fracture Mechanics*, 179:13–27, 2017.
- [19] Q. Zhao, A. Lisjak, O. Mahabadi, Q. Liu, and G. Grasselli. Numerical simulation of hydraulic fracturing and associated microseismicity using finite-discrete element method. *Journal of Rock Mechanics and Geotechnical Engineering*, 6(6):574–581, 2014.

(M. Xavier and A.A. Novotny) LABORATÓRIO NACIONAL DE COMPUTAÇÃO CIENTÍFICA LNCC/MCT, COORDENAÇÃO DE MATEMÁTICA APLICADA E COMPUTACIONAL, AV. GETÚLIO VARGAS 333, 25651-075 PETRÓPOLIS - RJ, BRASIL

E-mail address: {marcel,novotny}@lncc.br

(N. Van Goethem) UNIVERSIDADE DE LISBOA, FACULDADE DE CIÊNCIAS, DEPARTAMENTO DE MATEMÁTICA, CMAF+CIO, ALAMEDA DA UNIVERSIDADE, C6, 1749-016 LISBOA, PORTUGAL

E-mail address: vangoeth@fc.ul.pt