THERMO-MECHANICAL FRACTURE MODELING GOVERNED BY TOPOLOGICAL DERIVATIVES

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Abstract. In this work, the brittle crack nucleation and propagation process governed by a semi-coupled thermo-mechanical system in a quasi-static regime is investigated by using the topological derivative method. First, we write the Griffith-Francfort-Marigo Damage Model in the context of a thermo-mechanical problem. Then, the associated sensitivity with respect to the nucleation of a small damage, under the assumption of ideal thermal contact between the new crack lips, is presented. This result is used to devise a crack nucleation/propagation algorithm. In particular, the topological derivative field is used as descent direction to minimize the Francfort-Marigo shape functional indicating, in each iteration, the fracture nucleation and propagation path. The proposed topology optimization algorithm is able to capture the whole fracturing process, including important features of crack mechanics like kinking and bifurcations, as it is shown through some numerical experiments.

1. Introduction

Crack initiation and propagation phenomena induced by thermal effects have received significant attention in the literature owing to their relevance for many applications in mechanical and civil engineering problems. These applications encompass a diverse range of scenarios including thermal shock, concrete drying, thermal variation in composite materials, seasonal temperature variations, among others. Researchers have conducted numerous studies in this field, making significant contributions. For a comprehensive review of the developed methods, encompassing both experimental and numerical simulation approaches, refer to the introduction section of the work by Yan et al. (2021). Within this framework, a fundamental question concerns the prediction of paths described by one or multiple initial cracks during its propagation as well as the occurrence of new fractures (Allaire et al., 2011; Bittencourt et al., 1996; Bourdin et al., 2000; Maso and Iurlano, 2013; Van Goethem and Novotny, 2010). In general, one of the challenges in computational modeling of fractures consists of dealing with crack nucleation and propagation mechanisms, as well as in capturing complex fracture patterns such as kinking and bifurcations, by using a minimal number of user-defined algorithmic parameters (Xavier and Van Goethem, 2022).

As originally proposed by Van Goethem and Novotny (2010), and after confirmed by Xavier et al. (2017), the topological derivative method arises as a natural approach to deal with fracture modeling problems. The topological derivative method was rigorously introduced by Sokołowski and Żochowski (1999). Since then, it has been recognized as a powerful tool with applications in many areas of Physics and Engineering, including shape and topology optimization, inverse problems, imaging process, optimal design of micro structures, among others. For a comprehensive account of the topological derivative method, see the books by Novotny and Sokołowski (2013, 2020) and Novotny et al. (2019), for instance. See also the special issue on the topological derivative method and its applications in computational engineering recently published in the

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Engineering Computations Journal (Novotny et al., 2022), covering various topics ranging from new theoretical developments (Amstutz, 2022; Baumann and Sturm, 2022; Delfour, 2022) to applications in structural and fluid dynamics topology optimization (Kliewe et al., 2022; Romero, 2022; Santos and Lopes, 2022), geometrical inverse problems (Bonnet, 2022; Canelas and Roche, 2022; Fernandez and Prakash, 2022; Louër and Rapún, 2022a,b), synthesis and optimal design of metamaterials (Ferrer and Giusti, 2022; Yera et al., 2022), fracture mechanics modeling (Xavier and Van Goethem, 2022), up to industrial applications (Rakotondrainibe et al., 2022) and experimental validation of the topological derivative method (Barros et al., 2022).

The main idea from the work by Xavier et al. (2017) consists of minimizing the Griffith-Francfort-Marigo shape functional (Francfort and Marigo, 1993), with respect to the nucleation of a small damage, by using the topological derivative concept. In essence, the associated topological derivative field is used as descent direction in the minimization process indicating, in each iteration, the regions that have to be damaged. From this strategy, the resulting crack path is characterized by a sequence of inclusions representing the damaged areas. The entire methodology relies solely on a threshold approach driven by the topological derivative field, resulting in a striking simple algorithm able to capture crucial crack path features such as kinking and bifurcations. Several benchmark numerical simulations presenting all these features, including the famous Bittencourt's experiments (Bittencourt et al., 1996), were reproduced by Xavier et al. (2017). Since then, the proposed methodology has been successfully extended to address the process of fluid-driven crack propagation in permeable rocks, commonly known as *fracking* (Filho et al., 2022; Xavier et al., 2018, 2020), and to the context of brittle fracture modeling on Kirchhoff and Reissner-Mindlin plate bending models subject to bending and shear efforts (Xavier and Van Goethem, 2022). All these works, however, do not take into account the influence of thermal variations. Considering the crucial role of temperature changes in various real-world scenarios, it becomes imperative to extend the existing research to encompass this effect.

Therefore, in the present study, the topological derivative method is applied to investigate the brittle crack nucleation and propagation phenomena induced by thermal effects. First, we write the Griffith-Francfort-Marigo Damage Model in the context of a thermo-mechanical problem. After then, the associated sensitivity, with respect to the nucleation of a small damage, under the assumption of ideal thermal contact between the new crack surfaces, is presented. The resulting topological derivative field is used to devise a crack nucleation/propagation algorithm, similar to the one proposed by Xavier et al. (2017). The effectiveness of the present approach is demonstrated through some basic numerical experiments in the context of structures subjected to cooling effects.

The work is organized as follows. The thermo-mechanical model of fracture is introduced in Section 2. In Section 3, the associated topological derivative expression is obtained. The topology optimization algorithm is presented in Section 4. The numerical experiments are shown in Section 5. Finally, some concluding remarks are presented in Section 6.

2. Thermo-mechanical fracture model

In order to represent a body submitted to small variations of temperatures, let us consider an open and bounded geometric domain $\Omega \subset \mathbb{R}^2$ with Lipschitz boundary $\partial\Omega$. The domain Ω contains a subdomain $\omega \subset \Omega$, used to represent a pre-existing crack (see Figure 1). To characterize the damaged region, a parameter ρ defined as

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

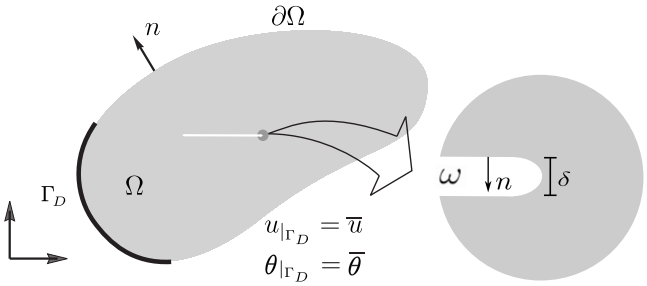

FIGURE 1. Cracked body submitted to small thermal variations.

with $0 < \rho_0 \ll 1$, is introduced. Therefore, the region $\Omega \setminus \overline{\omega}$ represents the undamaged part of the body and ω a thin damage.

From these elements, the main idea from the Griffith-Francfort-Marigo Damage Model (Francfort and Marigo, 1998, 1993) consists of minimizing a shape functional $\mathcal{F}_\omega(u,\theta)$ of the form

$$\mathcal{F}_\omega(u,\theta) = \mathcal{J}(u,\theta) + \kappa|\omega| \,, \tag{2.2}$$

with respect to the crack growth at the quasi-static time step t_i. The second term on the right hand side of (2.2) is the well-known Griffith's energy dissipation term while $\mathcal{J}(u,\theta)$, written as

$$\mathcal{J}(u,\theta) = \frac{1}{2}\int_\Omega \sigma(u)\cdot\varepsilon(u)\,dx - \int_\Omega Q(\theta)\cdot\varepsilon(u)\,dx \,, \tag{2.3}$$

is the total potential energy of the system for a given temperature θ. The displacement field u is solution to the variational problem

$$u \in \mathcal{U}^M : \int_\Omega \sigma(u)\cdot\varepsilon(\eta_u)\,dx = \int_\Omega Q(\theta)\cdot\varepsilon(\eta_u)\,dx \,,\ \forall \eta_u \in \mathcal{V}^M \,, \tag{2.4}$$

at the quasi-static time step t_i. In (2.4) the term $\sigma(\varphi)$ represents the Cauchy's stress tensor and is defined as

$$\sigma(\varphi) = \rho\mathbb{C}\varepsilon(\varphi) \,, \tag{2.5}$$

with the parameter ρ given by (2.1). We consider the body made of an isotropic material, so that the elasticity tensor $\mathbb{C}$ is written as

$$\mathbb{C} = 2\mu \mathrm{I}_4 + \lambda(\mathrm{I}_2 \otimes \mathrm{I}_2) \,, \tag{2.6}$$

where I_2 and I_4 are the second and fourth identity tensors, respectively, and μ and λ, given by

$$\mu = \frac{E}{2(1+\nu)} \quad \text{and} \quad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \,, \tag{2.7}$$

are the Lamé's coefficients for a structure under the plane strain assumption. The strain tensor, denoted by $\varepsilon(\varphi)$, is defined as

$$\varepsilon(\varphi) := \frac{1}{2}(\nabla\varphi + (\nabla\varphi)^\top) \,. \tag{2.8}$$

The set of admissible solutions to the elasticity problem, $\mathcal{U}^M$, and the associated variational space, $\mathcal{V}^M$, are defined as

$$\mathcal{U}^M := \left\{\phi \in H^1(\Omega;\mathbb{R}^2) : \phi|_{\Gamma_D} = \overline{u}\right\} , \tag{2.9}$$

$$\mathcal{V}^M := \left\{\phi \in H^1(\Omega;\mathbb{R}^2) : \phi|_{\Gamma_D} = 0\right\} , \tag{2.10}$$

respectively.

At the right hand side of (2.4), $Q(\theta)$ is the induced thermal stress tensor defined as

$$Q(\theta) = \beta\theta \mathrm{I}_2 \,, \tag{2.11}$$

where $\beta = \alpha\rho(2\mu + 3\lambda)$, with α used to denote the thermal expansion coefficient. The temperature field θ is solution to the following variational problem

$$\theta \in \mathcal{U}^T : \int_\Omega q(\theta) \cdot \nabla\eta_\theta \, dx = 0 \ , \ \forall \eta_\theta \in \mathcal{V}^T \ . \tag{2.12}$$

The heat flow $q(\theta)$ is defined as

$$q(\theta) = -\mathrm{K}\nabla\theta \ , \tag{2.13}$$

where K is a second-order tensor that represents the thermal conductivity of the medium. In the isotropic case, the tensor K can be written as

$$\mathrm{K} = k\mathrm{I}_2 \ , \tag{2.14}$$

with the thermal conductivity coefficient k defined by

$$k = k(x) := \begin{cases} k_m, & \text{if } x \in \Omega \setminus \overline{\omega} \ , \\ k_f, & \text{if } x \in \omega \ , \end{cases} \tag{2.15}$$

where k_m refers to the thermal conductivity of the matrix, while k_f to the thermal conductivity of the crack. Finally, the set $\mathcal{U}^T$ and the space $\mathcal{V}^T$ are, respectively, defined as

$$\mathcal{U}^T := \left\{ \phi \in H^1(\Omega; \mathbb{R}^2); \phi|_{\Gamma_D} = \overline{\theta}_i \right\} \ , \tag{2.16}$$

$$\mathcal{V}^T := \left\{ \phi \in H^1(\Omega; \mathbb{R}^2); \phi|_{\Gamma_D} = 0 \right\} \ , \tag{2.17}$$

where $\overline{\theta}_i$, given by

$$\overline{\theta}_i = \overline{\theta}_{i-1} + \Delta\overline{\theta}_i \ , \tag{2.18}$$

is the prescribed temperature on Γ_D at the pseudo time t_i with $\Delta\overline{\theta}_i$ used to denote the increment. Thus, the total prescribed temperature $\overline{\theta}$ is given by the sum

$$\overline{\theta} = \overline{\theta}_0 + \sum_{i=1}^{N} \Delta\overline{\theta}_i \ , \tag{2.19}$$

where $\overline{\theta}_0$ is the initial temperature and N is the number of increments. Notice that the temperature field θ and, consequently, the displacement field u, are induced by the boundary condition $\overline{\theta}_i$ prescribed on Γ_D at time t_i.

Taking into account the above described model, the minimization problem can be stated as: For each quasi-static time instant t_i,

$$\underset{\omega \subset \Omega}{\text{Minimize}} \ \ \mathcal{F}_\omega(u, \theta), \quad \text{subject to (2.4)} \ , \tag{2.20}$$

with $\mathcal{F}_\omega(u, \theta)$ given by (2.2).

Finally, in order to deal with the characterization of the critical thermal loading, the same strategy proposed by Xavier et al. (2018) is adopted here, i.e., the parameter κ is replaced by a new parameter κ_δ defined as

$$\kappa = \kappa_\delta := \frac{\kappa_s}{\delta} \ , \tag{2.21}$$

where κ_s represents a new material property and δ is the length of the initial damage.

As already mentioned, the topological derivative method arises as a natural tool to solve the minimization problem (2.20). In the following section, we provide the definition of this concept and present the resulting topological derivative field for the problem under consideration.

3. Topological derivative method

The topological derivative is defined as the first term of the asymptotic expansion of a given shape functional with respect to a small parameter that measures the size of singular domain perturbations, such as holes, inclusions, source-terms and cracks. In other words, the topological derivative measures the sensitivity of the associated shape functional with respect to the nucleation of a singular domain perturbation. See, for instance, the introductory book by Novotny and Sokołowski (2020).

The proposed approach involves evaluating the topological derivative of the shape functional (2.2) with respect to the nucleation of a small damage. In this study, considering the abrupt nature of the crack growth in brittle materials, we assume that the thermal contact between the new crack surfaces, during the fracture propagation process, is ideal. By employing this simplification, the topological sensitivity analysis does not take into account the influence of the thermal part. In this particular case, the resulting topological derivative field can be easily adapted from Xavier et al. (2020). The subsequent theorem presents this outcome, whose proof can be found in the paper by Xavier et al. (2020):

Theorem 1. *The topological derivative of the shape functional* (2.2)*, with respect to the nucleation of a small circular inclusion with different mechanical properties from the background, and under the assumption of ideal thermal contact between the new crack surfaces, is given by the sum*

$$D_T\mathcal{F}_\omega(x) = D_T\mathcal{J}(x) + \kappa_\delta \ , \quad \forall x \in \Omega \setminus \overline{\omega} \ , \tag{3.1}$$

with the first term $D_T\mathcal{J}(x)$ *written as*

$$D_T\mathcal{J}(x) = \mathbb{P}_0\sigma(u(x)) \cdot \varepsilon(u(x)) + (1+a)\beta\theta(x)\mathrm{div}(u)(x) - \frac{\beta^2\theta(x)^2}{2\mu} \ . \tag{3.2}$$

The polarization tensor $\mathbb{P}_0$ *is a fourth-order isotropic tensor given by*

$$\mathbb{P}_0 = -\frac{1+b}{2}\mathrm{I}_4 - \frac{a-b}{4}\mathrm{I}_2 \otimes \mathrm{I}_2 \ , \tag{3.3}$$

where the parameters a *and* b *are defined as*

$$a = \frac{\lambda+\mu}{\mu} \quad \textit{and} \quad b = \frac{\lambda+3\mu}{\lambda+\mu} \ , \tag{3.4}$$

respectively.

4. Topology optimization algorithm

The original algorithm proposed to study the process of crack nucleation/propagation based on the topological derivative field was presented by Xavier et al. (2017). The strategy consists of introducing an inclusion (small damage) at the regions where the topological derivative is negative. This approach is justified by noting that the introduction of an infinitesimal inclusion where the topological derivative is negative reduces the associated shape functional values. As a result, the crack path is identified by the sequence of inclusions that are nucleated during the minimization process. As highlighted in the previous section, fracture propagation in brittle materials is characterized by abrupt crack growth. Building upon this observation, we make the assumption that the thermal contact between the new fracture surfaces is ideal throughout the crack evolution, as mentioned earlier. In this scenario, from the algorithm standpoint, the pseudo time t_i and the corresponding temperature field remain fixed during crack propagation. In other words, only the material properties of the mechanical (elastic) system are updated based on the topological derivative. Once fracture propagation is completed, the pseudo time t_i

advances, and the semi-coupled thermo-mechanical system is then updated. The key elements of the original algorithm adapted to the present context are outlined as follows:

The size of the inclusion to be nucleated is associated with the region ω^* where the topological derivative is negative, i.e.,

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

Let $D_T\mathcal{F}_\omega^*$ be the minimum value of the topological derivative, i.e.,

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

The inclusion to be nucleated inside the region ω^*, denoted by ω^m, is defined as

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

where $m \in (0,1)$ is chosen in such a way that $|\omega^m| \approx \pi\delta^2/4$ (and $|\omega^m| \leq \pi\delta^2/4$) is satisfied, where δ represents the thickness of the initial damage. From these elements, the main steps of the modified algorithm can be summarized as follows:

(1) At a new pseudo time step, solve the thermal and the coupled elasticity problems;
(2) Evaluate the topological derivative field and check for the crack propagation criterion;
   (a) If the criterion is fulfilled, increase the damaged region according to the topological derivative, solve the elasticity system and go to (2);
   (b) Otherwise, return to (1).

Note that the Step (2), together with item (a), represent the crack propagation process. These steps are detailed below in the form of pseudo-code, see Algorithm 1. For more details concerning Algorithm 1, see the paper by Xavier et al. (2020).

Algorithm 1: Damage evolution algorithm.

Input : Ω, ω, δ, N, $\overline{\theta}_0$, $\Delta\overline{\theta}_i$
Output: Optimal topology $\omega^\star$

for $i = 1 : N$ **do**
  solve the thermal problem (2.12);
  solve the coupled elasticity system (2.4);
  evaluate the topological derivative $D_T\mathcal{F}_\omega$ according to (3.1);
  compute the threshold ω^* from (4.1);
  while $|\omega^*| \geq \pi\delta^2/4$ **do**
    intensify the mesh at the crack tip;
    solve the elasticity system (2.4);
    evaluate the topological derivative $D_T\mathcal{F}_\omega$ (3.1);
    compute the threshold ω^* from (4.1);
    compute the threshold ω^m from (4.3);
    nucleate a new inclusion ω^m inside ω^*;
    update the damaged region: $\omega \leftarrow \omega \cup \omega^m$;
    solve the elasticity system and evaluate $D_T\mathcal{F}_\omega$;
    evaluate the shape functional $\mathcal{F}_\omega$ from (2.2);
    if the shape functional increases, then break;
    else compute the threshold ω^*;
  end while
end for

5. Numerical Experiments

In the numerical examples, a cracked glass bar, fixed (clamped) on the supports by its vertical edges (homogeneous Dirichlet boundary conditions) and submitted to cooling (through the same edges), is represented by a reference domain Ω. The dimension of the bar is $(1 \times 0,5)m^2$ and the preexisting fracture is represented by an initial damage with length h and width δ, as shown in Figure 2. The location where fracture is expected to occur is identified by the distribution of elastic material (gray), and the compliant material (white) is used to represent the fracture. The structure, assumed to be under plane strain assumption, is fixed at the supports at temperature of $\overline{\theta}_0 = 275$°C and subjected to a cooling process up to the room temperature of $\overline{\theta} = 25$°C, with a variation of $\Delta\overline{\theta}_i = -2,5$°C at each time step, where $i = 1, \cdots, 100$. Note that in this case, the total temperature variation is -250°C, divided into $N = 100$ uniform increments. The used geometrical, thermal and mechanical parameters are shown in Table 1, where the parameter l represents the diameter of the inclusion. Finally, linear triangular finite elements are used to discretize the coupled thermo-mechanical system.

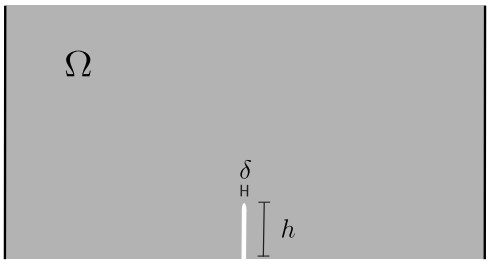

Figure 2. Cracked glass bar submitted to cooling effects.

Table 1. Parameters.

Parameter	Value	Parameter	Value
h	0,1 m	E	75 GPa
δ	0,005 m	ρ_0	10^{-6}
l	$(2/3)\delta$	ν	0,24
$\Delta\overline{\theta}_i$	$-2,5$ °C	κ_s	2×10^3 J/m
k_m	0,8 W/m°C	α_m	$9,0 \times 10^{-6}$ °C^{-1}
k_f	0,03 W/m°C	α_f	$1/273$ °C^{-1}

5.1. **Homogeneous medium.** In this initial example, we consider the glass bar to be a perfectly homogeneous medium. In this case, the fracture propagates in a straight line, as expected; the final material distribution is presented in Figure 3. Note that the thermal effects induce the first opening mode. The observed thermal critical temperature is $\overline{\theta}_c = 247,5$°C. The history of the shape functional can be seen in Figure 4. Note that the model dissipates energy in all iterations.

5.2. **Heterogeneous medium.** In the second example, an heterogeneous medium is considered. In this case, the Young's modulus E is corrupted with White Gaussian Noise (WGN) of zero mean and standard deviation τ. Therefore, the parameter E is replaced by $E_\tau = E(1+\tau s)$, where $s : \Omega \to \mathbb{R}$ is a function assuming random values in the interval $(0,1)$ and $\tau = 2,5$ corresponds to the noise level. The used parameters are the same of the previous example.

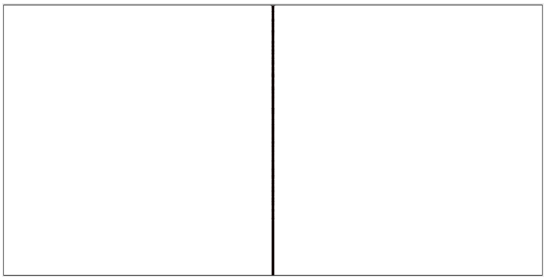

FIGURE 3. Homogeneous medium: obtained crack path.

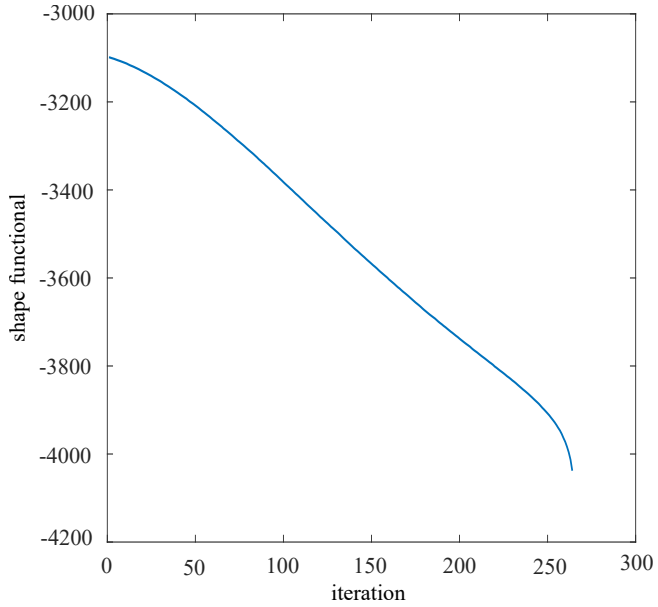

FIGURE 4. Homogeneous medium: history of the shape functional

Figure 5 shows the corrupted Young's modulus E_τ. The crack evolution, associated with each observed critical temperature, can be seen in Figures 6 and 7. Note that, due to the medium heterogeneity, we can observe kinking and bifurcations phenomena, which is more aligned with expected physical behavior.

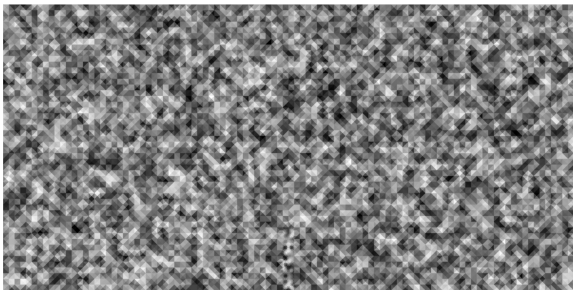

FIGURE 5. Heterogeneous medium: Corrupted Young's modulus E_τ.

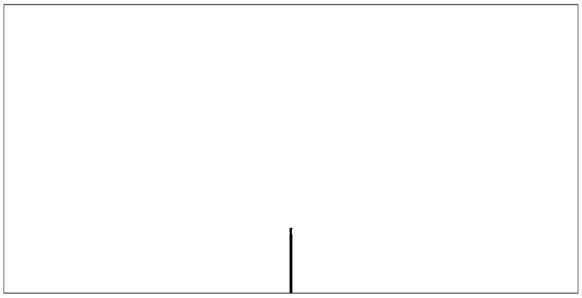

FIGURE 6. Heterogeneous medium: Obtained crack path at $\overline{\theta} = 207,5°\text{C}$.

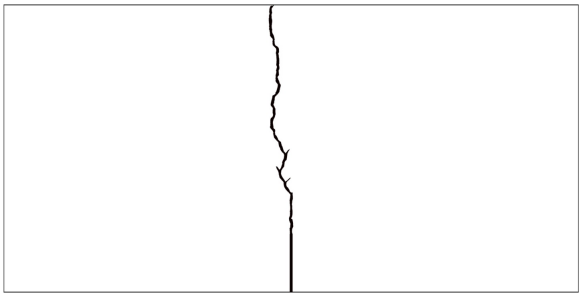

FIGURE 7. Heterogeneous medium: Obtained crack path $\overline{\theta} = 205°\text{C}$.

6. Conclusion

In this study, we propose a numerical scheme in order to investigate the brittle crack nucleation and propagation phenomena induced by thermal effects. A semi-coupled thermo-mechanical problem, considering the presence of a pre-existing fracture, was modeled by using the well-known Francfort-Marigo damage model. By assuming ideal thermal contact between the new fracture surfaces during the crack growth, the associated topological derivative, with respect to the nucleation of a small damage, was obtained. The resulting topological derivative field was then used to devise a crack nucleation/propagation algorithm, similar to the one proposed by Xavier et al. (2017). To assess the effectiveness of our approach, we conducted basic numerical experiments focused on structures subjected to cooling effects. These experiments successfully capture crucial fracture modeling features in brittle materials, including kinking and bifurcations. These results demonstrate the robustness and applicability of our methodology.

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