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RESEARCH PAPER

Topological sensitivity analysis in large deformation problems

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Abstract The aim of the present work is to apply the topological sensitivity analysis (TSA) to large-deformation elasticity based on the total Lagrangian formulation. The TSA results in a scalar function, denominated topological derivative, that gives for each point of the domain the sensitivity of a given cost function when a small hole is created. An approximated expression for the topological derivative is obtained by numerical asymptotic analysis. Numerical results of the presented approach are considered for elastic plane problems.

Keywords Topological optimization · Finite element method · Linear and nonlinear elasticity · Sensitivity analysis · Topological derivative

1 Introduction

The topological optimization techniques obtain the optimal shape of a given structure, which minimizes the objective function and restrictions of the physical problem without any information about the initial shape of the structural domain. Topological optimization may be classified as discrete and continuous. For discrete structures, the optimal topology is determined by the optimal number, position, and connectivity of the structural elements. A complete review of discrete topological optimization may be found in Rozvany et al. (1995), Rozvany (1997), Bendsϕe (1995), Eschenauer et al. (1982), Olhoff and Rozvany (1995), and Gutkowski and Mroz (1997).

The topological optimization of continuous structures may be classified in the material (micro) and geometrical (macro) approaches. The main technique of the material approach is the solid isotropic microstructures with penalization (SIMP) (Bendsϕe 1995, 1989; Rozvany and Zhou 1991; Rozvany et al. 1992; Zhou and Rozvany 1991; Bendsϕe and Sigmund 1999). The methods evolutionary structural optimization (ESO) and topological sensitivity analysis (TSA) are techniques related to the geometrical approach (Zhao et al. 1997; Novotny et al. 2003). In the SIMP method, a density field $\rho(\mathbf{x}) \in [0, 1]$ is defined as the design variable and the total derivatives are calculated in the classical form. For the ESO method, an approximated sensitivity is calculated based on the finite difference of the objective function when an element of the mesh is removed (Zhao et al. 1997). The TSA technique calculates the sensitivity of the cost function when a small hole is created in the domain of the problem (Novotny et al. 2003). The sensitivity is described by the topological derivative or gradient.

The topological derivative has been determined for the steady-state heat conduction problem and 2D and 3D linear elasticity problems (Novotny et al. 2003; Novotny 2003). For the nonlinear case, the topological derivative is obtained for the nonlinear torsion problem of a primastic bar under stationary fluency described by the p-Poisson equation (Novotny et al. 2005a). The TSA concept has not been applied yet to nonlinear vector problems.

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The purpose of this work is to present the application of the TSA to large deformation elastic problems. Initially, the concept of topological derivative is presented, as well as a brief description of the large deformation problem. The TSA is defined for the large deformation problem and the total Lagrangian formulation. The TSA is applied to the total potential energy functional, and the expression of the topological derivative is obtained. An asymptotic numerical analysis is developed to study the behavior of the analytical expression of the topological derivative. Despite the fact that the topological derivative is just an indicator of the sensitivity of the functional when a small hole is created in the problem domain, a heuristic topological optimization algorithm may be defined. Finally, the algorithm is applied to large-deformation planar structures and conclusions are addressed.

2 Definition of topological derivative

The topological derivative is a scalar function defined in the whole domain of the problem definition. It gives the sensitivity of a cost function when a small hole is created in the neighborhood of a point (Garreau et al. 1998; Novotny et al. 2003). In the original definition of the topological derivative (Garreau et al. 1998), after the creation of the hole, it is no longer possible to establish a homeomorfism between the perturbed domain (with the hole) and the unperturbed one (without the hole).

Consider the domains Ω and $\Omega_\varepsilon \in \Re^n$, where $\Omega_\varepsilon = \Omega - \bar{B}_\varepsilon$. The boundary of Ω_ε is denoted by $\Gamma_\varepsilon = \Gamma \cup \partial B_\varepsilon$, and $\bar{B}_\varepsilon = B_\varepsilon \cup \partial B_\varepsilon$ is a ball of radius ε centered in $\hat{\mathbf{x}} \in \Omega$ with a measure that tends to zero when $\varepsilon \to 0$. In this way, Ω represents the unperturbed domain (without the hole) and Ω_ε represents the perturbed domain (with a small hole) as it can be seen in Fig. 1. The original definition of the topological derivative for a cost function ψ can be mathematically written in the following way (Masmoudi 1998):

$$D_T^*\left(\hat{\mathbf{x}}\right) = \lim_{\varepsilon \to 0} \frac{\psi\left(\Omega_\varepsilon\right) - \psi\left(\Omega\right)}{f\left(\varepsilon\right)}, \tag{1}$$

being $f(\varepsilon)$ a negative monotonically decreasing regularizing function in such a way that $f(\varepsilon) \to 0$ when $\varepsilon \to 0$ $(0 \leq \varepsilon < 1)$, and it will depend on the problem being analyzed. This definition is illustrated in Fig. 1. The considered domains do not have the same topology. Due to this fact, the derivative (1) cannot be calculated in the conventional way.

A new definition of the topological derivative is presented in Novotny et al. (2003). The idea is to start from a problem where the hole B_ε already exists. From that, a mapping between the domains $\Omega_\varepsilon \in \Re^n$ and $\Omega_{\varepsilon+\delta\varepsilon} \in \Re^n$ is defined, being $\delta\varepsilon$ a variation of the radius ε of B_ε, which results in the hole $B_{\varepsilon+\delta\varepsilon}$ in $\Omega_{\varepsilon+\delta\varepsilon}$. Based on that, it is possible to define a new perturbed domain $\Omega_{\varepsilon+\delta\varepsilon} = \Omega - \bar{B}_{\varepsilon+\delta\varepsilon}$, where the boundary can be written as $\Gamma_{\varepsilon+\delta\varepsilon} = \Gamma \cup \partial B_{\varepsilon+\delta\varepsilon}$, as illustrated in Fig. 2. In this way, it is established a continuous and one-to-one mapping between Ω_ε and $\Omega_{\varepsilon+\delta\varepsilon}$ that has a continuous inverse. Therefore, Ω_ε and $\Omega_{\varepsilon+\delta\varepsilon}$ become homeomorphic. Then, the topological derivative can be redefined in the following way:

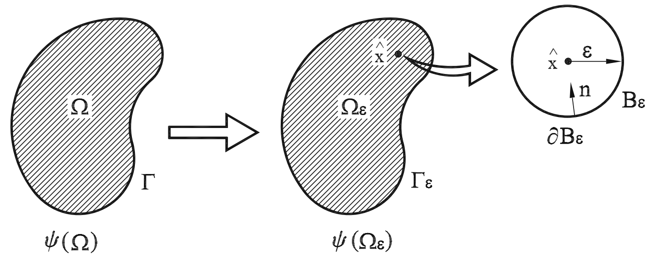

Fig. 1 Original definition of the topological derivative, Novotny et al. (2003)

$$D_T\left(\hat{\mathbf{x}}\right) = \lim_{\substack{\varepsilon \to 0 \\ \delta\varepsilon \to 0}} \frac{\psi\left(\Omega_{\varepsilon+\delta\varepsilon}\right) - \psi\left(\Omega_\varepsilon\right)}{f\left(\varepsilon+\delta\varepsilon\right) - f\left(\varepsilon\right)}. \tag{2}$$

The new definition of the topological derivative gives the sensitivity of the cost function ψ when the hole B_ε, centered at the point $\hat{\mathbf{x}}$ and with $\varepsilon \to 0$, increases in size and not when this is effectively created according to the original definition (1). However, expanding a hole of radius ε when $\varepsilon \to 0$ is equivalent to creating it. The action of increasing a hole B_ε can be interpreted as a sequence of configurations denoted by the parameter τ. If the domain suffers a perturbation (increasing the hole), this can be interpreted by a smooth and invertible mapping, which depends on the parameter τ, defined as $\mathcal{X}(\mathbf{x},\tau)$ with $\mathbf{x} \in \Omega_\varepsilon \subset \Re^n$ and $\tau \in \Re$. The sequence of domains Ω_τ and the perturbed boundaries Γ_τ can be defined, respectively, as $\Omega_\tau = \{\mathbf{x}_\tau \in \Re^n \,|\, \exists \mathbf{x} \in \Omega_\varepsilon, \mathbf{x}_\tau = \mathcal{X}(\mathbf{x},\tau)\}$ and $\Gamma_\tau = \{\mathbf{x}_\tau \in \Re^n \,|\, \exists \mathbf{x} \in \Gamma_\varepsilon, \mathbf{x}_\tau = \mathcal{X}(\mathbf{x},\tau)\}$, $(\mathbf{x}_\tau|_{\tau=0} = \mathbf{x}$, $\Gamma_\tau|_{\tau=0} = \Gamma_\varepsilon$, $\Omega_\tau|_{\tau=0} = \Omega_\varepsilon)$.

In this way, the domain $\Omega_{\varepsilon+\delta\varepsilon}$, perturbed by a smooth expansion $\delta\varepsilon$ of the ball B_ε, and its respective boundary $\Gamma_{\varepsilon+\delta\varepsilon}$ can be written with relation to τ as $\Omega_{\varepsilon+\delta\varepsilon} = \Omega_\tau \Longrightarrow \Omega_\varepsilon = \Omega_\tau|_{\tau=0}$ and $\Gamma_{\varepsilon+\delta\varepsilon} = \Gamma_\tau \Longrightarrow \Gamma_\varepsilon = \Gamma_\tau|_{\tau=0}$.

For τ sufficiently small, the mapping $\mathbf{x}_\tau = \mathcal{X}(\mathbf{x},\tau)$ between the domains is written as

$$\mathbf{x}_\tau = \mathbf{x} + \tau\mathbf{v}\left(\mathbf{x}\right), \tag{3}$$

where $\mathbf{x} = \mathcal{X}(\mathbf{x},0)$ and $\mathbf{v}(\mathbf{x}) = \frac{\partial\mathcal{X}(\mathbf{x},0)}{\partial\tau}$ is a shape design change. According to Zolézio (1981), only the

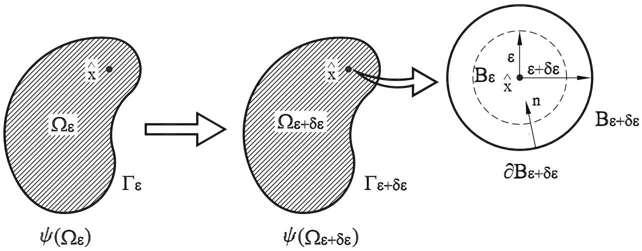

Fig. 2 Modified definition of the topological derivative, Novotny et al. (2003)

component of the velocity field $\mathbf{v}$ in the normal direction to the boundary Γ_ε, denoted by v_n, is meaningful in the sensitivity calculations. Therefore,

$$\mathbf{x}_\tau = \mathbf{x} + \tau v_n \mathbf{n}, \quad \forall\, \mathbf{x} \in \partial B_\varepsilon. \tag{4}$$

It is possible to associate the perturbation $\delta\varepsilon$ with the parameter τ ($\forall\, \mathbf{x} \in \partial B_\varepsilon$ and $\forall\, \mathbf{x}_\tau \in \partial B_{\varepsilon+\delta\varepsilon}$) as

$$\delta\varepsilon = \|\mathbf{x}_\tau - \mathbf{x}\| = \|\tau v_n \mathbf{n}\| = \tau\, |v_n|\,. \tag{5}$$

Based on the above definitions, the equivalence between the topological derivative definitions given by (1) and (2) can be formalized as Novotny et al. (2003)

$$D_T^*\left(\hat{\mathbf{x}}\right) = D_T\left(\hat{\mathbf{x}}\right) = \frac{1}{|v_n|} \lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \left.\frac{d\psi\left(\Omega_\tau\right)}{d\tau}\right|_{\tau=0}. \tag{6}$$

3 Large deformation problems

In a large deformation problem, the final configuration of the body $\Omega \in \Re^n$ can differ greatly from the initial configuration or the reference configuration $\Omega^0 \in \Re^n$. A body is deformed through a one-to-one mapping $\mathbf{f}$ that relates each material point $\mathbf{X} \in \Omega^0$ to a point $\mathbf{x} \in \Omega$ in such a way that $\mathbf{x} = \mathbf{f}(\mathbf{X}) \in \Omega$ and $\det \nabla\mathbf{f} > 0$. The vector $\mathbf{u}(\mathbf{X}) = \mathbf{f}(\mathbf{X}) - \mathbf{X}$ represents the displacement of the point $\mathbf{X}$.

The stress–strain relation for the generalized Hooke law and the total Lagrangian formulation can be written as follows:

$$\mathbf{S} = \mathsf{C} : \mathbf{E}, \tag{7}$$

where $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor, $\mathbf{E}$ is the finite Green-Lagrange deformation tensor and $\mathbf{E} = \nabla\mathbf{u}^S + \frac{1}{2}\nabla\mathbf{u}^T\nabla\mathbf{u}$, C is the material elasticity tensor and $\mathsf{C} = 2\bar{\mu}\mathsf{I} + \bar{\lambda}\left(\mathbf{I}\otimes\mathbf{I}\right)$ with $\bar{\mu}$ and $\bar{\lambda}$ the Lamé constants, and I is the fourth-order unitary tensor.

It is assumed that the reference domain $\Omega^0 \in \Re^n$ is open and bounded. Its boundary $\Gamma^0 = \Gamma_N^0 \cup \Gamma_D^0$, $\left(\Gamma_D^0 \cap \Gamma_N^0 = \emptyset\right)$ is sufficiently regular and admits the existence of a normal unitary vector $\mathbf{n}$ in almost all of the points of Γ^0, except in a finite set of zero measure.

The variational problem for the case of large deformations and homogeneous isotropic linear and elastic material is given by the virtual work principle as follows: find $\mathbf{u} \in \mathcal{U}$, such that

$$a\left(\mathbf{u},\delta\mathbf{u}\right) = l\left(\delta\mathbf{u}\right), \quad \forall\, \delta\mathbf{u} \in \mathcal{V}, \tag{8}$$

where $\mathcal{U} = \left\{\mathbf{u} \in \left[H^1\left(\Omega^0\right)\right]^{\dim} \mid \mathbf{u}|_{\Gamma_D^0} = \bar{\mathbf{u}}\right\}$, $\mathcal{V} = \left\{\delta\mathbf{u} \in \left[H^1\left(\Omega^0\right)\right]^{\dim} \mid \delta\mathbf{u}|_{\Gamma_D^0} = \mathbf{0}\right\}$ and $\dim \le 3$. The abstract form $a\left(\mathbf{u},\delta\mathbf{u}\right)$ is bounded and linear in $\delta\mathbf{u}$ but nonlinear in $\mathbf{u}$; $l\left(\delta\mathbf{u}\right)$ is a limited and linear form. Such forms can be written in the following way (Bonet and Wood 1997):

$$a\left(\mathbf{u},\delta\mathbf{u}\right) = \int_{\Omega^0} \mathbf{S}\cdot\delta\mathbf{E}\, d\Omega^0 = \int_{\Omega^0} \mathsf{C} : \mathbf{E}\cdot\delta\mathbf{E}\, d\Omega^0\,, \tag{9}$$

$$l\left(\delta\mathbf{u}\right) = \int_{\Omega^0} \mathbf{b}_0\cdot\delta\mathbf{u}\, d\Omega^0 + \int_{\Gamma_N^0} \mathbf{t}_0\cdot\delta\mathbf{u}\, d\Gamma^0\,, \tag{10}$$

where $\mathbf{b}_0$ is a sufficiently smooth vector in the reference configuration Ω^0 that represents the body forces, $\mathbf{t}_0$ is a vector in the reference configuration that represents the applied load in the Neumann boundary Γ_N^0, and $\delta\mathbf{u}$ is the virtual displacement. The term $\delta\mathbf{E}$ in (9) represents a virtual variation of the tensorial strain field and is related to $\delta\mathbf{u}$ through the following relation (Belytschko et al. 2001; Bonet and Wood 1997):

$$\begin{aligned}\delta\mathbf{E} &= \frac{1}{2}\left(\mathbf{F}^T\delta\mathbf{F} + \delta\mathbf{F}^T\mathbf{F}\right) \\ &= \nabla\delta\mathbf{u}^S + \frac{1}{2}\left(\nabla\delta\mathbf{u}^T\nabla\mathbf{u} + \nabla\mathbf{u}^T\nabla\delta\mathbf{u}\right).\end{aligned} \tag{11}$$

4 TSA for the total Lagrangian formulation

The concept of topological derivative can be applied to large deformation problems described with the total Lagrangian formulation. Consider a new domain $\Omega_\varepsilon^0 \in \Re^n$, $\Omega_\varepsilon^0 = \Omega^0 - \bar{B}_\varepsilon^0$, that has a boundary denoted by $\Gamma_\varepsilon^0 = \Gamma^0 \cup \partial B_\varepsilon^0$ and $\bar{B}_\varepsilon^0 = B_\varepsilon^0 \cup \partial B_\varepsilon^0$ is a ball of radius ε and centered at the material point $\hat{\mathbf{X}} \in \Omega_\varepsilon^0$, as illustrated in Fig. 3.

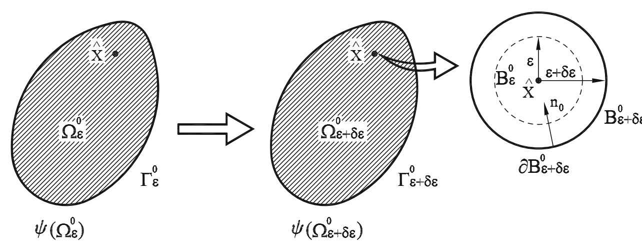

Fig. 3 Modified definition of the topological derivative for the total Lagrangian formulation

From (2), a total Lagrangian description for the topological derivative can be written as

$$D_T(\hat{\mathbf{X}}) = \lim_{\substack{\varepsilon \to 0 \\ \delta\varepsilon \to 0}} \frac{\psi\left(\Omega^0_{\varepsilon+\delta\varepsilon}\right) - \psi\left(\Omega^0_\varepsilon\right)}{f(\varepsilon+\delta\varepsilon) - f(\varepsilon)}. \tag{12}$$

The above equation represents the sensitivity of the cost function when the hole B^0_ε, centered at the material point $\hat{\mathbf{X}} \in \Omega^0_\varepsilon$ and with radius $\varepsilon \to 0$, increases in size and not when this is effectively created, as in the original definition (1) of the topological derivative

The action of increasing a hole can be interpreted as a sequence of perturbed configurations characterized by the parameter τ and described by a smooth and invertible function $\mathcal{T}(\mathbf{X}, \tau)$ with $\mathbf{X} \in \Omega^0_\varepsilon \subset \Re^n$ and $\tau \in \Re$. In this way, the sequence of domains Ω^0_τ and respective perturbed reference boundaries Γ^0_τ can be defined as $\Omega^0_\tau = \{\mathbf{X}_\tau \in \Re^n | \exists\, \mathbf{X} \in \Omega^0_\varepsilon, \mathbf{X}_\tau = \mathcal{T}(\mathbf{X}, \tau), \mathbf{X}_\tau|_{\tau=0} = \mathbf{X}\}$ and $\Gamma^0_\tau = \left\{\mathbf{X}_\tau \in \Re^n | \exists\, \mathbf{X} \in \Gamma^0_\varepsilon, \mathbf{X}_\tau = \mathcal{T}(\mathbf{X}, \tau)\right\}$, where $\Omega^0_\tau\big|_{\tau=0} = \Omega^0_\varepsilon$ and $\Gamma^0_\tau\big|_{\tau=0} = \Gamma^0_\varepsilon$. In this way, the domain $\Omega^0_{\varepsilon+\delta\varepsilon}$, perturbed by a smooth expansion $\delta\varepsilon$ of the ball B^0_ε, and its respective boundary $\Gamma^0_{\varepsilon+\delta\varepsilon}$ can be written with relation to τ as $\Omega^0_{\varepsilon+\delta\varepsilon} = \Omega^0_\tau \Longrightarrow \Omega^0_\varepsilon = \Omega^0_\tau\big|_{\tau=0}$ and $\Gamma^0_{\varepsilon+\delta\varepsilon} = \Gamma^0_\tau \Longrightarrow \Gamma^0_\varepsilon = \Gamma^0_\tau\big|_{\tau=0}$.

The mapping between the unperturbed reference domain Ω^0_ε and the perturbed domain Ω^0_τ can be written as

$$\mathbf{X}_\tau = \mathbf{X} + \tau V_n \mathbf{n}_0, \quad \forall\, \mathbf{X} \in \partial B^0_\varepsilon, \tag{13}$$

where V_n is the normal component to the hole of the velocity field $\mathbf{V}$ in the reference configuration. Analogous to (5), the perturbation $\delta\varepsilon$ is associated to the parameter τ in the following way ($\forall\, \mathbf{X} \in \partial B^0_\varepsilon$ and $\forall\, \mathbf{X}_\tau \in \partial B^0_{\varepsilon+\delta\varepsilon}$):

$$\delta\varepsilon = \|\mathbf{X}_\tau - \mathbf{X}\| = \|\tau V_n \mathbf{n}_0\| = \tau\, |V_n|. \tag{14}$$

Considering that the domain used in the shape variation sensitivity is the reference domain Ω^0, then (6) can be rewritten as

$$D^*_T(\hat{\mathbf{X}}) = D_T(\hat{\mathbf{X}}) = \frac{1}{|V_n|} \lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} \left.\frac{d\psi\left(\Omega^0_\tau\right)}{d\tau}\right|_{\tau=0}, \tag{15}$$

where $D^*_T(\hat{\mathbf{X}})$ is the original topological derivative defined between the reference domain without the hole Ω^0 and the reference domain with the hole Ω^0_ε; $D_T\left(\hat{\mathbf{X}}\right)$ is the modified topological derivative given by (12), and $f(\varepsilon)$ is the regularizing function chosen in such a away that $0 < \left|D^*_T(\hat{\mathbf{X}})\right| < \infty$.

5 Total potential energy functional for large deformation

Considering that the domain Ω^0_ε is bounded and open and that Γ^0_ε is sufficiently regular, then the variational problem defined by equation (8) in Ω^0 can be redefined in the unperturbed reference domain Ω^0_ε in the following way: find $\mathbf{u}_\varepsilon \in \mathcal{U}_\varepsilon$ such that

$$a_\varepsilon(\mathbf{u}_\varepsilon, \delta\mathbf{u}_\varepsilon) = l_\varepsilon(\delta\mathbf{u}_\varepsilon), \quad \forall\, \delta\mathbf{u}_\varepsilon \in \mathcal{V}_\varepsilon, \tag{16}$$

where $\mathcal{U}_\varepsilon = \left\{\mathbf{u}_\varepsilon \in \left[H^1(\Omega_\varepsilon)\right]^{\dim} | \mathbf{u}_\varepsilon|_{\Gamma_D} = \bar{\mathbf{u}}\right\}$ and $\mathcal{V}_\varepsilon = \left\{\eta_\varepsilon \in \left[H^1(\Omega_\varepsilon)\right]^{\dim} | \eta_\varepsilon|_{\Gamma_D} = \mathbf{0}\right\}$ are, respectively, the spaces of the cinematically admissible displacements and admissible variations in the domain of dimension $\dim \leq 3$; $H^1(\Omega_\varepsilon)$ is the Sobolev space of the functions with first derivative integrable in the Lebesgue sense; and $\bar{\mathbf{u}}$ is the prescribed displacement over the Dirichlet boundary Γ_D. According to (9) and (10), the abstract form of (16) can be rewritten in the following way:

$$\int_{\Omega^0_\varepsilon} \mathbf{S}_\varepsilon \cdot \delta\mathbf{E}_\varepsilon \, d\Omega^0_\varepsilon = \int_{\Omega^0_\varepsilon} \mathbf{b}_0 \cdot \delta\mathbf{u}_\varepsilon \, d\Omega^0_\varepsilon + \int_{\Gamma^0_N} \mathbf{t}_0 \cdot \delta\mathbf{u}_\varepsilon \, d\Gamma^0. \tag{17}$$

In an analogous manner, the variational problem in the perturbed reference domain Ω^0_τ is given by to following: find $\mathbf{u}_\tau \in \mathcal{U}_\tau$, such that

$$a_\tau(\mathbf{u}_\tau, \delta\mathbf{u}_\tau) = l_\tau(\delta\mathbf{u}_\tau), \quad \forall\, \delta\mathbf{u}_\tau \in \mathcal{V}_\tau \text{ and } \forall\, \tau \geq 0, \tag{18}$$

where $\mathcal{U}_\tau$ and $\mathcal{V}_\tau$ are the spaces of functions and variations, respectively, defined in Ω^0_τ.

The total potential energy functional $\Psi_\tau(\mathbf{u}_\tau)$ is defined in the following manner:

$$\Psi_\tau(\mathbf{u}_\tau) = \frac{1}{2} \int_{\Omega^0_\tau} \mathbf{S}_\tau \cdot \mathbf{E}_\tau \, d\Omega^0_\tau \tag{19}$$

$$- \int_{\Omega_\tau} \mathbf{b}_0 \cdot \mathbf{u}_\tau \, d\Omega^0_\tau - \int_{\Gamma_N} \mathbf{t}_0 \cdot \mathbf{u}_\tau \, d\Gamma^0_\tau$$

$$= \frac{1}{2} a_\tau(\mathbf{u}_\tau, \mathbf{u}_\tau) - l_\tau(\mathbf{u}_\tau). \tag{20}$$

Based on the shape sensitivity analysis, the sensitivity of the cost function (20), with relation to the perturbation created by the velocity field in (13), is characterized by the total derivative of $\Psi_\tau(\mathbf{u}_\tau)$ with relation to τ in $\tau = 0$ given by

$$\left.\frac{d\Psi_\tau(\mathbf{u}_\tau)}{d\tau}\right|_{\tau=0} = \lim_{\tau \to 0} \frac{\Psi_\tau(\mathbf{u}_\tau) - \Psi_0(\mathbf{u}_0)}{\tau}, \tag{21}$$

where $\mathbf{u}_\tau$ is an implicit function of τ through the state equation (18) and $\mathbf{u}_0 = \mathbf{u}_\tau|_{\tau=0} = \mathbf{u}_\varepsilon$ is a solution of the state equation (16) defined in the unperturbed configuration Ω_ε.

Formally, the calculation of the total derivative of $\Psi_\tau(\mathbf{u}_\tau)$ with relation to τ in $\tau = 0$ is the total derivative of $\Psi_\tau(\mathbf{u}_\tau)$ over the tangent plane for the restriction given by the state equation (Novotny et al. 2003)

$$\begin{cases} \text{Calculate:} & \left.\frac{d\Psi_\tau(\mathbf{u}_\tau)}{d\tau}\right|_{\tau=0} \\ \text{Subject to:} & a_\tau(\mathbf{u}_\tau, \eta_\tau) = l_\tau(\eta_\tau) \end{cases}. \tag{22}$$

To obtain the sensitivity of the cost function (20), the Lagrangian for the nonlinear problem in the perturbed configuration Ω_τ^0 is written in the following way:

$$L_\tau(\mathbf{u}_\tau, \beta_\tau) = \Psi_\tau(\mathbf{u}_\tau) + a_\tau(\mathbf{u}_\tau, \beta_\tau) - l_\tau(\beta_\tau), \forall\, \beta_\tau \in \mathcal{V}_\tau. \tag{23}$$

The abstract formulation $a_\tau(\mathbf{u}_\tau, \delta\mathbf{u}_\tau)$ of (18) is nonlinear in $\mathbf{u}_\tau$ and linear in $\delta\mathbf{u}_\tau$. Therefore, $\beta_\tau = m\,\delta\mathbf{u}_\tau$, where $m \in \Re$ is the Lagrange multiplier for the equality restriction $a_\tau(\mathbf{u}_\tau,\delta\mathbf{u}_\tau) - l_\tau(\delta\mathbf{u}_\tau) = 0$ in the Lagrangian function (23) and $\beta_\tau \in \mathcal{V}_\tau$.

Considering that (18) is satisfied for every τ, then the total derivative of the Lagrangian function (23) will be equal to the derivative of the total potential energy function, that is

$$\frac{dL_\tau}{d\tau} = \frac{d\Psi_\tau}{d\tau} = \frac{\partial L_\tau}{\partial\tau} + \left\langle \frac{\partial L_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle + \left\langle \frac{\partial L_\tau}{\partial\beta_\tau}, \dot{\beta}_\tau \right\rangle \tag{24}$$

with $\dot{\mathbf{u}}_\tau = \frac{d\mathbf{u}_\tau}{d\tau} \in \mathcal{V}_\tau$ and $\dot{\beta}_\tau = \frac{d\beta_\tau}{d\tau} \in \mathcal{V}_\tau$.

Taking into account that, in (23), the functional $\Psi_\tau(\mathbf{u}_\tau)$ and the abstract form $a_\tau(\mathbf{u}_\tau, \beta_\tau)$ depend explicitly of $\mathbf{u}_\tau$, then the directional derivative $\left\langle \frac{\partial L_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle$ in equation (24) can be written as

$$\left\langle \frac{\partial L_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle = \left\langle \frac{\partial \Psi_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle + \left\langle \frac{\partial a_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle. \tag{25}$$

The β_τ-dependence of $a_\tau(\mathbf{u}_\tau, \beta_\tau)$ and $l_\tau(\beta_\tau)$ implies that the directional derivative $\left\langle \frac{\partial L_\tau}{\partial\beta_\tau}, \dot{\beta}_\tau \right\rangle$ is given as

$$\left\langle \frac{\partial L_\tau}{\partial\beta_\tau}, \dot{\beta}_\tau \right\rangle = \left\langle \frac{\partial a_\tau}{\partial\beta_\tau}, \dot{\beta}_\tau \right\rangle - \left\langle \frac{\partial l_\tau}{\partial\beta_\tau}, \dot{\beta}_\tau \right\rangle. \tag{26}$$

Considering that, for the problem in question, $a_\tau(\mathbf{u}_\tau, \beta_\tau)$ is defined according to equation (9), the directional derivative of the abstract form $a_\tau(\mathbf{u}_\tau, \beta_\tau)$ with relation to $\mathbf{u}_\tau$ in the direction $\dot{\mathbf{u}}_\tau$ becomes

$$\left\langle \frac{\partial a_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle = \int_{\Omega_\tau^0} \mathsf{C} : \left\langle \frac{\partial \mathbf{E}_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle \cdot \delta\mathbf{E}_\tau + \mathbf{S}_\tau \cdot \left\langle \frac{\partial \delta\mathbf{E}_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle d\Omega_\tau^0$$
$$= \delta a_\tau(\mathbf{u}_\tau; \dot{\mathbf{u}}_\tau, \beta_\tau). \tag{27}$$

The derivatives of the Green–Lagrange deformation tensor $\mathbf{E}_\tau$, and also the derivatives of its variation $\delta\mathbf{E}_\tau$ with relation to $\mathbf{u}_\tau$ in the direction $\dot{\mathbf{u}}_\tau$, are expressed, respectively, as

$$\left\langle \frac{\partial \mathbf{E}_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle = \nabla_\tau\dot{\mathbf{u}}_\tau^S + \frac{1}{2}\nabla_\tau\mathbf{u}_\tau^T\nabla_\tau\dot{\mathbf{u}}_\tau + \frac{1}{2}\nabla_\tau\dot{\mathbf{u}}_\tau^T\nabla_\tau\mathbf{u}_\tau, \tag{28}$$

$$\left\langle \frac{\partial \delta\mathbf{E}_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle = \frac{1}{2}\nabla_\tau\dot{\mathbf{u}}_\tau^T\nabla_\tau\beta_\tau + \frac{1}{2}\nabla_\tau\beta_\tau^T\nabla_\tau\dot{\mathbf{u}}_\tau. \tag{29}$$

The variation of the Green–Lagrange deformation tensor is expressed in relation to $\mathbf{u}_\tau$ and $\delta\mathbf{u}_\tau$ as

$$\delta\mathbf{E}_\tau = \nabla_\tau\delta\mathbf{u}_\tau^S + \frac{1}{2}\nabla_\tau\mathbf{u}_\tau^T\nabla_\tau\delta\mathbf{u}_\tau + \frac{1}{2}\nabla_\tau\delta\mathbf{u}_\tau^T\nabla_\tau\mathbf{u}_\tau. \tag{30}$$

On the other hand, the directional derivative of the abstract form $a_\tau(\mathbf{u}_\tau, \beta_\tau)$ with relation to β_τ in the direction $\dot{\beta}_\tau$ is

$$\left\langle \frac{\partial a_\tau}{\partial\beta_\tau}, \dot{\beta}_\tau \right\rangle = \int_{\Omega_\tau^0} \mathbf{S}_\tau \cdot \left[\nabla_\tau\dot{\beta}_\tau^S + \frac{1}{2}\nabla_\tau\mathbf{u}_\tau^T\nabla_\tau\dot{\beta}_\tau + \frac{1}{2}\nabla_\tau\dot{\beta}_\tau^T\nabla_\tau\mathbf{u}_\tau \right] d\Omega_\tau^0 = a_\tau\left(\mathbf{u}_\tau, \dot{\beta}_\tau\right). \tag{31}$$

Similarly, the directional derivative of the linear term $l_\tau(\beta_\tau)$ with relation to β_τ in the direction $\dot{\beta}_\tau$ becomes

$$\left\langle \frac{\partial l_\tau}{\partial\beta_\tau}, \dot{\beta}_\tau \right\rangle = \int_{\Omega_\tau^0} \mathbf{b}_0 \cdot \dot{\beta}_\tau\, d\Omega_\tau^0 + \int_{\Gamma_N^0} \mathbf{t}_0 \cdot \dot{\beta}_\tau\, d\Gamma_\tau^0$$
$$= l_\tau\left(\dot{\beta}_\tau\right). \tag{32}$$

The calculation of the partial derivative of the Lagrangian function $L_\tau(\mathbf{u}_\tau, \beta_\tau)$ with relation to τ will coincide with the calculation of the total derivative with relation to τ if

$$\left\langle \frac{\partial L_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle = \left\langle \frac{\partial \Psi_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle + \delta a_\tau(\mathbf{u}_\tau; \dot{\mathbf{u}}_\tau, \beta_\tau) = 0, \tag{33}$$

$$\left\langle \frac{\partial L_\tau}{\partial\beta_\tau}, \dot{\beta}_\tau \right\rangle = a_\tau\left(\mathbf{u}_\tau, \dot{\beta}_\tau\right) - l_\tau\left(\dot{\beta}_\tau\right) = 0, \tag{34}$$

Remembering the symmetry of the bilinear form $\delta a_\tau(\mathbf{u}_\tau; \dot{\mathbf{u}}_\tau, \beta_\tau)$, (33) resumes to the following problem: find $\beta_\tau \in \mathcal{V}_\tau$, such that

$$\delta a_\tau(\mathbf{u}_\tau; \beta_\tau, \dot{\mathbf{u}}_\tau) = -\left\langle \frac{\partial \Psi_\tau}{\partial\mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle, \quad \forall\, \dot{\mathbf{u}}_\tau \in \mathcal{V}_\tau. \tag{35}$$

Analogously, (34) is equivalent to the state equation of the following problem: find $\mathbf{u}_\tau \in \mathcal{U}_\tau$, such that

$$a_\tau\left(\mathbf{u}_\tau, \dot{\beta}_\tau\right) = l_\tau\left(\dot{\beta}_\tau\right), \quad \forall\, \dot{\beta}_\tau \in \mathcal{V}_\tau. \tag{36}$$

Therefore, if $\mathbf{u}_\tau$ and β_τ are, respectively, solutions of (36) and (35), then the following relation is valid:

$$\frac{\partial L_\tau(\mathbf{u}_\tau, \beta_\tau)}{\partial\tau} = \left.\frac{dL_\tau(\mathbf{u}_\tau, \beta_\tau)}{d\tau}\right|_{\mathbf{u}_\tau \text{ and } \beta_\tau \text{ fixed}}. \tag{37}$$

Taking the directional derivative of $\Psi_\tau(\mathbf{u}_\tau)$ with relation to $\mathbf{u}_\tau$ in the direction $\dot{\mathbf{u}}_\tau$ and considering the symmetry of $a_\tau(\mathbf{u}_\tau, \mathbf{u}_\tau)$ [according to (35)], then

$$\left\langle \frac{\partial \Psi_\tau(\mathbf{u}_\tau)}{\partial \mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle = \frac{1}{2}\left\langle \frac{\partial a_\tau(\mathbf{u}_\tau, \mathbf{u}_\tau)}{\partial \mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle - \left\langle \frac{\partial l_\tau(\mathbf{u}_\tau)}{\partial \mathbf{u}_\tau}, \dot{\mathbf{u}}_\tau \right\rangle = a_\tau(\mathbf{u}_\tau, \dot{\mathbf{u}}_\tau) - l_\tau(\dot{\mathbf{u}}_\tau). \tag{38}$$

Considering that the body force vector $\mathbf{b}_0$ and the surface force vector $\mathbf{t}_0$ do not depend on $\mathbf{u}_\tau$, then

$$a_\tau(\mathbf{u}_\tau, \dot{\mathbf{u}}_\tau) = \int_{\Omega_\tau^0} \mathsf{C} : \mathbf{E}_\tau \cdot \left(\nabla_\tau \dot{\mathbf{u}}_\tau^S + \frac{1}{2}\nabla_\tau \mathbf{u}_\tau^T \nabla_\tau \dot{\mathbf{u}}_\tau + \frac{1}{2}\nabla_\tau \dot{\mathbf{u}}_\tau^T \nabla_\tau \mathbf{u}_\tau \right) d\Omega_\tau^0, \tag{39}$$

$$l_\tau(\dot{\mathbf{u}}_\tau) = \int_{\Omega_\tau^0} \mathbf{b}_0 \cdot \dot{\mathbf{u}}_\tau \, d\Omega_\tau^0 + \int_{\Gamma_N^0} \mathbf{t}_0 \cdot \dot{\mathbf{u}}_\tau \, d\Gamma_\tau^0. \tag{40}$$

For $\dot{\mathbf{u}}_\tau \in \mathcal{V}_\tau$, (39) and (40) are equivalent to (9) and (10) written in the perturbed configuration Ω_τ^0 and changing $\delta\mathbf{u}$ by $\dot{\mathbf{u}}_\tau$. Consequently, (39) and (40) represent the state equation of the problem so that the adjoint equation (35) can be written as

$$\delta a_\tau(\mathbf{u}_\tau; \beta_\tau, \dot{\mathbf{u}}_\tau) = a_\tau(\mathbf{u}_\tau, \dot{\mathbf{u}}_\tau) - l_\tau(\dot{\mathbf{u}}_\tau) = 0, \ \forall\, \dot{\mathbf{u}}_\tau \in \mathcal{V}_\tau. \tag{41}$$

In this way, the solution of the auxiliary problem for the total potential energy function and the problem being considered is $\beta_\tau = \mathbf{0}$.

Based on relation (37), the definition of the total potential energy functional (20), and considering that the solution of the auxiliary equation is $\beta_\tau = \mathbf{0}$, the partial derivative of the Lagrangian (23), written in the unperturbed configuration $\Omega_\tau^0\big|_{\tau=0} = \Omega_\varepsilon^0$, is

$$\left.\frac{\partial L_\tau}{\partial \tau}\right|_{\tau=0} = \frac{1}{2}\left.\frac{\partial a_\tau(\mathbf{u}_\tau, \mathbf{u}_\tau)}{\partial \tau}\right|_{\tau=0} - \left.\frac{\partial l_\tau(\mathbf{u}_\tau)}{\partial \tau}\right|_{\tau=0}. \tag{42}$$

Applying Reynolds transport theorem (Gurtin 1981), the partial derivative, in the unperturbed configuration Ω_ε^0, of the abstract form $a_\tau(\mathbf{u}_\tau, \mathbf{u}_\tau)$ is given by

$$\begin{aligned}\left.\frac{\partial a_\tau(\mathbf{u}_\tau, \mathbf{u}_\tau)}{\partial \tau}\right|_{\tau=0} &= \int_{\Omega_\varepsilon^0} \left[\left.\frac{\partial (\mathbf{S}_\tau \cdot \mathbf{E}_\tau)}{\partial \tau}\right|_{\tau=0} + (\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon)\ \mathrm{Div}\mathbf{V} \right] d\Omega_\varepsilon^0 \\ &= 2\int_{\Omega_\varepsilon^0} \left[\mathsf{C} : \mathbf{E}_\tau \cdot \left.\frac{\partial (\mathbf{E}_\tau)}{\partial \tau}\right|_{\tau=0} + \frac{1}{2}(\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon)\,\mathbf{I} \cdot \nabla\mathbf{V} \right] d\Omega_\varepsilon^0. \end{aligned} \tag{43}$$

The derivative of the Green–Lagrange deformation tensor can be rewritten in the following manner:

$$\left.\frac{\partial (\mathbf{E}_\tau)}{\partial \tau}\right|_{\tau=0} = \left.\frac{\partial \left(\nabla_\tau \mathbf{u}_\tau^S\right)}{\partial \tau}\right|_{\tau=0} + \frac{1}{2}\left.\frac{\partial \left(\nabla_\tau \mathbf{u}_\tau^T\right)}{\partial \tau}\right|_{\tau=0} \nabla\mathbf{u}_\tau + \frac{1}{2}\nabla\mathbf{u}_\tau^T \left.\frac{\partial (\nabla_\tau \mathbf{u}_\tau)}{\partial \tau}\right|_{\tau=0}. \tag{44}$$

Taking into consideration the fact that the state equations (36) and the adjoint equation (35) are satisfied (i.e., $\mathbf{u}_\tau$ and β_τ are fixed), the partial derivative of the gradient of the vector field $\mathbf{u}_\tau$ with relation to τ, in the unperturbed configuration, is (Novotny et al. 2003)

$$\left.\frac{\partial (\nabla\mathbf{u}_\tau)}{\partial \tau}\right|_{\tau=0} = -\nabla\mathbf{u}_\varepsilon \nabla\mathbf{V}. \tag{45}$$

For the equivalent symmetric gradient

$$\left.\frac{\partial \left(\nabla\mathbf{u}_\tau^S\right)}{\partial \tau}\right|_{\tau=0} = -\left(\nabla\mathbf{u}_\varepsilon \nabla\mathbf{V}\right)^S. \tag{46}$$

Therefore, the partial derivative of the deformation tensor $\mathbf{E}_\tau$ in the unperturbed configuration is

$$\left.\frac{\partial (\mathbf{E}_\tau)}{\partial \tau}\right|_{\tau=0} = -\left(\nabla\mathbf{u}_\varepsilon \nabla\mathbf{V}\right)^S - \frac{1}{2}\left(\nabla\mathbf{u}_\varepsilon \nabla\mathbf{V}\right)^T \nabla\mathbf{u}_\varepsilon - \frac{1}{2}\nabla\mathbf{u}_\varepsilon^T \nabla\mathbf{u}_\varepsilon \nabla\mathbf{V}. \tag{47}$$

Substituting (47) in (43) and after algebraic manipulations, the partial derivative of a_τ with relation to τ in the unperturbed configuration can be written as

$$\left.\frac{\partial a_\tau(\mathbf{u}_\tau, \mathbf{u}_\tau)}{\partial \tau}\right|_{\tau=0} = 2\int_{\Omega_\varepsilon^0} \left[\frac{1}{2}(\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon)\,\mathbf{I} - \nabla\mathbf{u}_\varepsilon^T \mathbf{S}_\varepsilon - \nabla\mathbf{u}_\varepsilon^T \nabla\mathbf{u}_\varepsilon \mathbf{S}_\varepsilon \right] \cdot \nabla\mathbf{V} \, d\Omega_\varepsilon^0. \tag{48}$$

Analogously, the partial derivative of the linear form $l_\tau(\mathbf{u}_\tau)$ with relation to τ in the unperturbed configuration $\tau = 0$ for $\mathbf{u}_\tau$ and β_τ fixed is

$$\left.\frac{\partial l_\tau(\mathbf{u}_\tau)}{\partial \tau}\right|_{\tau=0} = \int_{\Omega_\varepsilon^0} (\mathbf{b}_0 \cdot \mathbf{u}_\varepsilon)\ \mathrm{Div}\mathbf{V}\, d\Omega_\varepsilon^0 + \int_{\Gamma_N^0} (\mathbf{t}_0 \cdot \mathbf{u}_\varepsilon)\ \mathrm{Div}_\Gamma\mathbf{V}\, d\Gamma^0, \tag{49}$$

where the surface divergent of the velocity field $\mathbf{V}$ is given by

$$\mathrm{Div}_\Gamma = (\mathbf{I} - \mathbf{n}_0 \otimes \mathbf{n}_0) \cdot \nabla\mathbf{V}. \tag{50}$$

As $\mathbf{V} = \mathbf{0}$ in Γ^0, then $\mathrm{Div}_\Gamma\mathbf{V} = 0$. Therefore,

$$\left.\frac{\partial l_\tau(\mathbf{u}_\tau)}{\partial \tau}\right|_{\tau=0} = \int_{\Omega_\varepsilon^0} (\mathbf{b}_0 \cdot \mathbf{u}_\varepsilon)\,\mathbf{I} \cdot \nabla\mathbf{V}\, d\Omega_\varepsilon^0. \tag{51}$$

Substituting the derivative of the abstract forms given by (48) and (51) in (42) and after algebraic manipulations, the partial derivative of the Lagrangian in $\tau = 0$ is

$$\left.\frac{\partial L_\tau}{\partial \tau}\right|_{\tau=0} = \int_{\Omega_\varepsilon^0}\left[\frac{1}{2}\left(\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon - 2\mathbf{b}_0 \cdot \mathbf{u}_\varepsilon\right)\mathbf{I} - \nabla\mathbf{u}_\varepsilon^T\mathbf{S}_\varepsilon - \nabla\mathbf{u}_\varepsilon^T\nabla\mathbf{u}_\varepsilon\mathbf{S}_\varepsilon\right] \cdot \nabla\mathbf{V}\, d\Omega_\varepsilon^0 . \quad (52)$$

The above equation can be written in the following manner:

$$\left.\frac{\partial L_\tau}{\partial \tau}\right|_{\tau=0} = \int_{\Omega_\varepsilon^0} \Sigma_\varepsilon^0 \cdot \nabla\mathbf{V}\, d\Omega_\varepsilon^0 , \quad (53)$$

where Σ_ε^0 represents the Eshelby energy moment tensor in the reference configuration for the total Lagrangian formulation. It is denoted as

$$\Sigma_\varepsilon^0 = \frac{1}{2}\left(\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon - 2\mathbf{b}_0 \cdot \mathbf{u}_\varepsilon\right)\mathbf{I} - \nabla\mathbf{u}_\varepsilon^T\mathbf{S}_\varepsilon - \nabla\mathbf{u}_\varepsilon^T\nabla\mathbf{u}_\varepsilon\mathbf{S}_\varepsilon . \quad (54)$$

Using the relations $\mathbf{P} = \mathbf{FS}$ and $\mathbf{F} = \mathbf{I} + \nabla\mathbf{u}$, the Eshelby tensor can be written in the following, more compact form:

$$\begin{aligned}\Sigma_\varepsilon^0 &= \frac{1}{2}\left(\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon - 2\mathbf{b}_0 \cdot \mathbf{u}_\varepsilon\right)\mathbf{I} - \nabla\mathbf{u}_\varepsilon^T\mathbf{S}_\varepsilon - \nabla\mathbf{u}_\varepsilon^T\left(\mathbf{F}_\varepsilon - \mathbf{I}\right)\mathbf{S}_\varepsilon \\ &= \frac{1}{2}\left(\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon - 2\mathbf{b}_0 \cdot \mathbf{u}_\varepsilon\right)\mathbf{I} - \nabla\mathbf{u}_\varepsilon^T\mathbf{P}_\varepsilon . \end{aligned} \quad (55)$$

The relation $W_\varepsilon = \frac{1}{2}\mathbf{P}_\varepsilon \cdot \mathbf{F}_\varepsilon = \frac{1}{2}\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon$ represents the energy density in the unperturbed reference configuration Ω_ε^0, (see Belytschko et al. 2001; Holzapfel 2000). Based on that, (55) can be rewritten as

$$\Sigma_\varepsilon^0 = \frac{1}{2}\left(\mathbf{P}_\varepsilon \cdot \mathbf{F}_\varepsilon - 2\mathbf{b}_0 \cdot \mathbf{u}_\varepsilon\right)\mathbf{I} - \nabla\mathbf{u}_\varepsilon^T\mathbf{P}_\varepsilon . \quad (56)$$

Applying the divergence theorem (Gurtin 1981) and the tensor relation

$$\Sigma_\varepsilon^0 \cdot \nabla\mathbf{V} = \mathrm{Div}\left[\left(\Sigma_\varepsilon^0\right)^T\mathbf{V}\right] - \mathrm{Div}\left(\Sigma_\varepsilon^0\right) \cdot \mathbf{V}, \quad (57)$$

(53) becomes

$$\left.\frac{\partial L_\tau}{\partial \tau}\right|_{\tau=0} = \int_{\Omega_\varepsilon^0} \mathrm{Div}\left(\Sigma_\varepsilon^0\right) \cdot \mathbf{V}\, d\Omega_\varepsilon^0 + \int_{\Gamma_\varepsilon^0} \Sigma_\varepsilon^0\mathbf{n}_0 \cdot \mathbf{V}\, d\Gamma_\varepsilon^0 . \quad (58)$$

It is possible to show that (Pereira 2006)

$$\mathrm{Div}\Sigma_\varepsilon^0 = \mathbf{0}. \quad (59)$$

Substituting (59) in (58) and considering the definition of the velocity field, then

$$\left.\frac{\partial L_\tau}{\partial \tau}\right|_{\tau=0} = -V_n \int_{\partial B_\varepsilon^0} \Sigma_\varepsilon^0\mathbf{n}_0 \cdot \mathbf{n}_0\, d\partial B_\varepsilon^0 . \quad (60)$$

From (55),

$$\Sigma_\varepsilon^0\mathbf{n}_0 \cdot \mathbf{n}_0 = \frac{1}{2}\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon - \mathbf{b}_0 \cdot \mathbf{u}_\varepsilon - \mathbf{P}_\varepsilon\mathbf{n}_0 \cdot \left(\nabla\mathbf{u}_\varepsilon\right)\mathbf{n}_0 .$$

Considering homogeneous Neumann boundary condition on the hole, that is, $\mathbf{P}_\varepsilon\mathbf{n}_0 = \mathbf{0}$ over ∂B_ε^0, and the absence of body forces $\mathbf{b}_0 = \mathbf{0}$, then

$$\left.\frac{\partial L_\tau}{\partial \tau}\right|_{\tau=0} = -V_n \int_{\partial B_\varepsilon^0} \left(\frac{1}{2}\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon\right) d\partial B_\varepsilon^0 . \quad (61)$$

The topological derivative is obtained by substituting (61) in expression (15). Therefore,

$$\begin{aligned} D_T^*\left(\hat{\mathbf{x}}\right) &= D_T\left(\hat{\mathbf{x}}\right) \\ &= -\lim_{\varepsilon\to 0} \frac{1}{f'(\varepsilon)} \int_{\partial B_\varepsilon^0} \left(\frac{1}{2}\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon\right) d\partial B_\varepsilon^0 . \end{aligned} \quad (62)$$

6 Numerical asymptotic analysis

Equation (63) represents the topological derivative, except for the limit with $\varepsilon \to 0$, for the case of large deformations and linear homogeneous and isotropic material. Therefore, to obtain the topological derivative, it is necessary that the limit for $\varepsilon \to 0$ in (63) be calculated either analytical or approximately. For the present nonlinear problem, an asymptotic analysis of (63) becomes impracticable because, in this case, it is not possible to obtain an analytical solution for the problem as described in the references Novotny et al. (2003, 2005b). An alternative procedure based on numerical experiments for the calculation of the limit with $\varepsilon \to 0$ in (63) is adopted as suggested in Novotny et al. (2003).

Consider the function $d_T\left(\mathbf{u}_\varepsilon\right)$ defined by

$$d_T\left(\mathbf{u}_\varepsilon\right) = -\frac{1}{f'(\varepsilon)} \int_{\partial B_\varepsilon^0} \left(\frac{1}{2}\mathbf{S}_\varepsilon \cdot \mathbf{E}_\varepsilon\right) d\partial B_\varepsilon^0 , \quad (63)$$

in such a way that

$$D_T\left(\hat{\mathbf{X}}\right) = \lim_{\varepsilon\to 0} d_T\left(\mathbf{u}_\varepsilon\right) . \quad (64)$$

A numerical study of the asymptotic behavior of the function $d_T\left(\mathbf{u}_\varepsilon\right)$ with relation to the radius ε is developed. Consider a plane rectangular domain, denoted by Ω, with dimensions $L = 2$ mm and with a hole of radius ε at the center of the domain subjected to the distributed load cases $\mathbf{t}_0$ along the side edges of Ω, as illustrated in Fig. 4. Symmetry conditions in the planes x and y are considered. It is assumed to be a plane strain model, with Poisson coefficient $\nu = 1/4$ and a Young modulus $E = 2,100$ N/mm^2.

The finite element meshes of quadratic triangles are constructed in such a way that they have the same

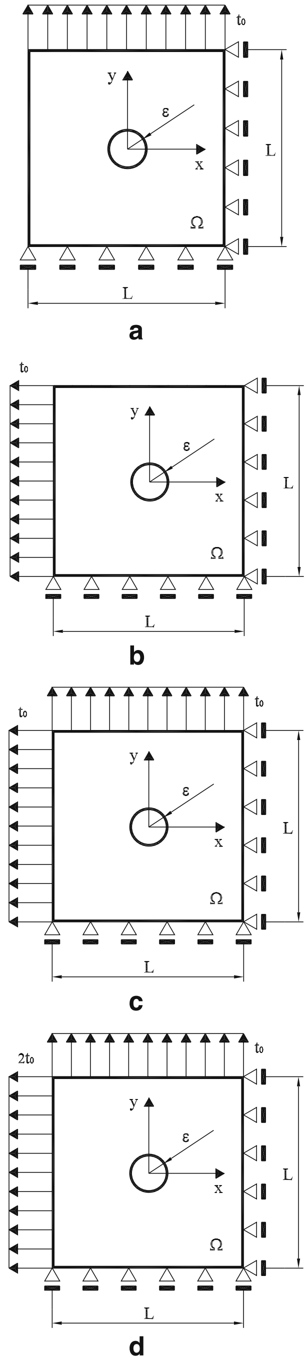

Fig. 4 Models used in the asymptotic analysis. **a** First case model. **b** Second case model. **c** Third case model. **d** Fourth case model

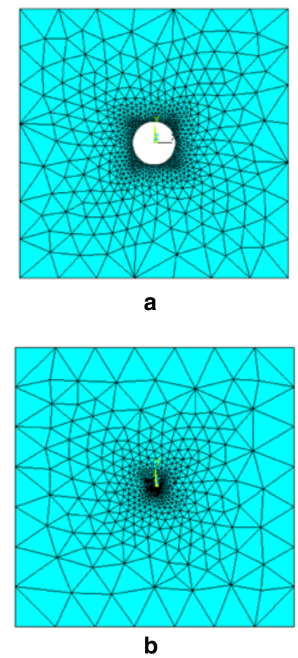

Fig. 5 Finite element meshes used in the asymptotic analysis. **a** Mesh with hole of $\varepsilon = 0.16$ mm. **b** Mesh without hole

number of elements at the boundary of the hole, independently of the value of the radius ε (Fig. 5). Consequently, the approximated size of the elements is calculated as

$$h^e \approx \frac{2\pi\varepsilon}{n_e}, \tag{65}$$

n_e being the number of elements required over the boundary of the hole. Table 1 shows the total number of elements N_E of the meshes generated in the domain Ω for different values of the radius ε and $n_e = 60$.

The plots $d_T(\mathbf{u}_\varepsilon)\, f'(\varepsilon) \times \varepsilon$ for $\mathbf{t}_0 = \pm\{12.50; 25.00; 37.50; 150.00; 450.00\}$ N/mm^2 are shown in Figs. 6 and 7, respectively, for the cases of traction and compression. It was not possible to obtain the solution for the compression load of $\mathbf{t}_0 = 450.00$ N/mm^2 because of the excessive distortion of the mesh.

Based on the analysis of the plots, it is reasonable to assume that these behave as straight lines that cross the origin. Consequently, the integrand in (63) behaves like a constant in relation to ε. A function $f(\varepsilon)$ that satisfies the condition $0 < \left|D_T\left(\hat{\mathbf{X}}\right)\right| < \infty$ is $f(\varepsilon) = -|B_\varepsilon| = -\pi\varepsilon^2$.

Table 1 Meshes used in the numerical asymptotic analysis

ε [mm]	N_E
0.01	3, 876
0.02	1, 968
0.03	1, 846
0.04	1, 760
0.05	1, 672
0.06	1, 644
0.07	1, 592
0.08	1, 576
0.10	1, 480
0.12	1, 408
0.16	1, 296

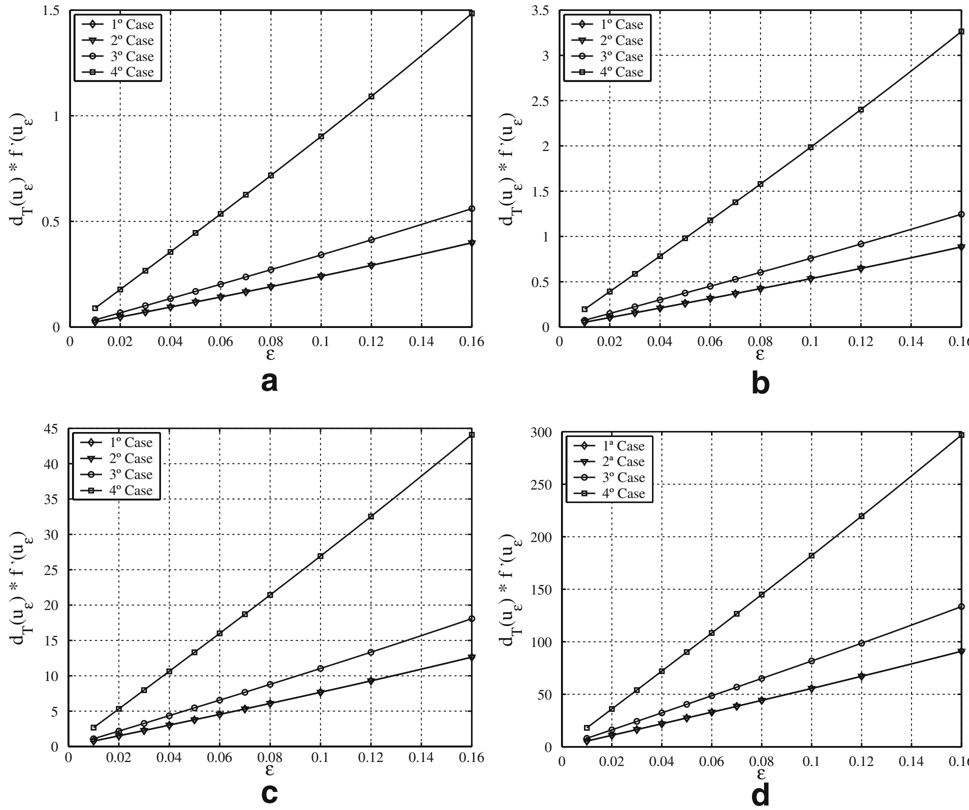

Fig. 6 Asymptotic behavior of $d_T(\mathbf{u}_\varepsilon)\, f'(\varepsilon)$ in terms of ε in the large deformation traction problem. **a** Load $\mathbf{t}_0 = 25.00$ N/mm^2. **b** Load $\mathbf{t}_0 = 37.50$ N/mm^2. **c** Load $\mathbf{t}_0 = 150.00$ N/mm^2. **d** Load $\mathbf{t}_0 = 450.00$ N/mm^2

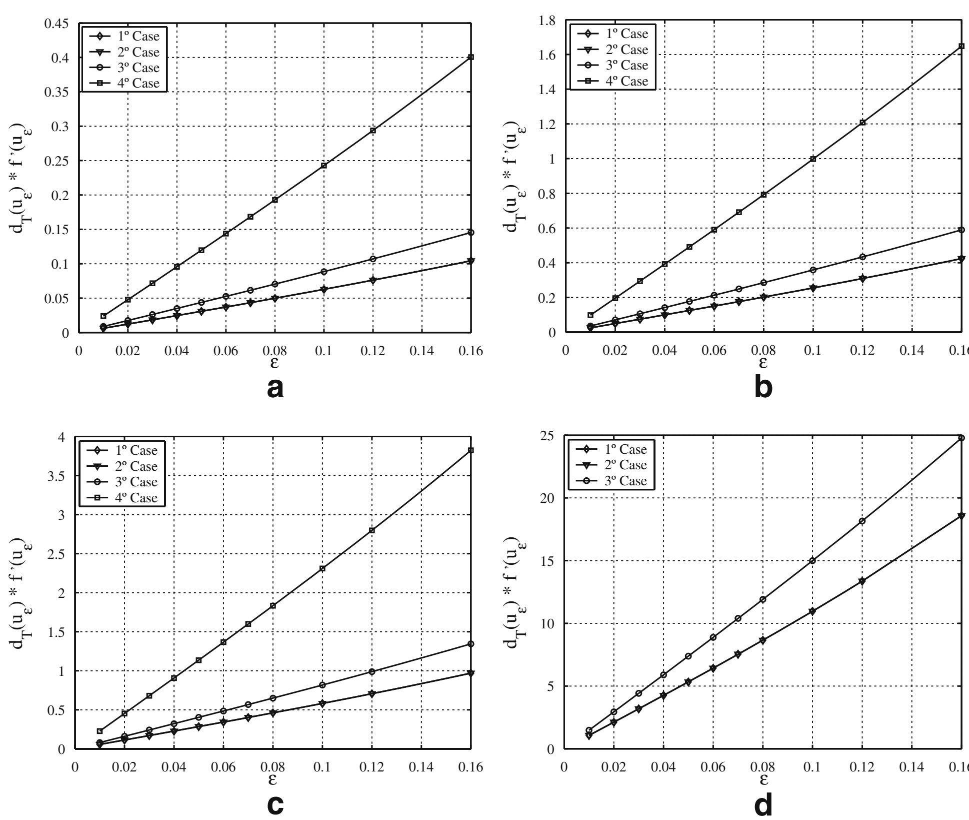

Fig. 7 Asymptotic behavior of $d_T(\mathbf{u}_\varepsilon)\, f'(\varepsilon)$ in terms of ε in the large deformation compression problem. **a** Load $\mathbf{t}_0 = -12.50$ N/mm^2. **b** Load $\mathbf{t}_0 = -25.00$ N/mm^2. **c** Load $\mathbf{t}_0 = -37.50$ N/mm^2. **d** Load $\mathbf{t}_0 = -150.00$ N/mm^2

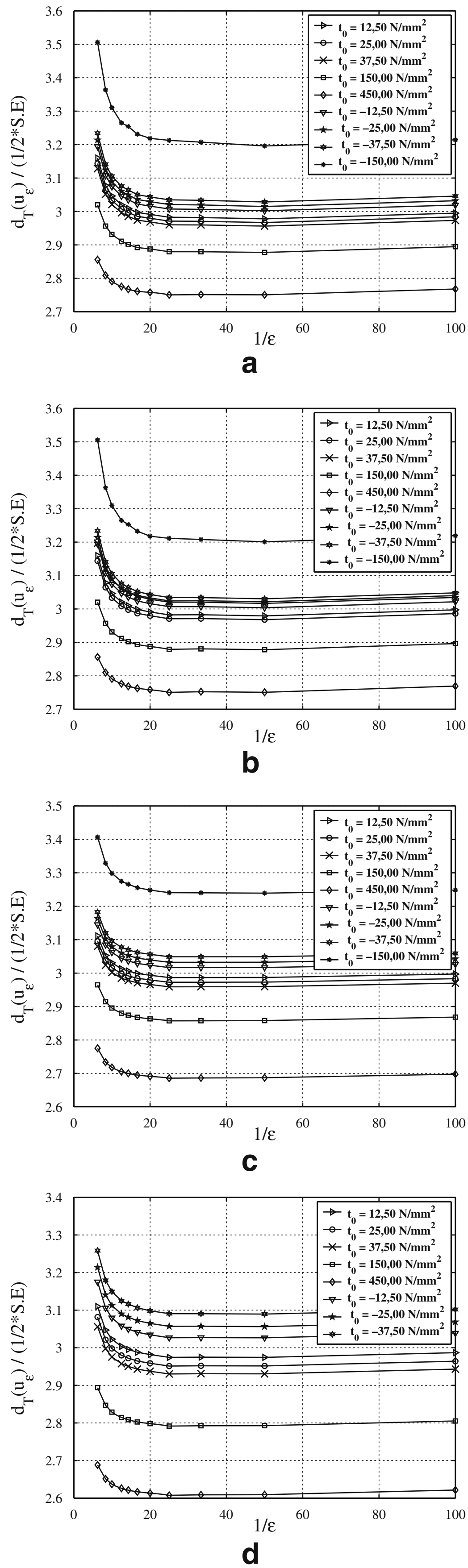

Fig. 8 Asymptotic behavior of the quotient $\frac{d_T(\mathbf{u}_\varepsilon)}{\frac{1}{2}\mathbf{S}\cdot\mathbf{E}}$ in relation to ε. **a** First load case. **b** Second load case. **c** Third load case. **d** Fourth load case

Consequently, (64) and (63) lead to

$$D_T(\hat{\mathbf{X}}) = \lim_{\varepsilon\to 0} d_T(\mathbf{u}_\varepsilon) = C\frac{1}{2}\mathbf{S}\cdot\mathbf{E}, \tag{66}$$

where C is a constant. Therefore, (66) is the final expression of the topological derivative, except for a constant.

The analysis of the constant C is performed through the asymptotic behavior of the function $d_T(\mathbf{u}_\varepsilon)$ in relation to the radius ε. Such analysis is based on the quotient between the function $d_T(\mathbf{u}_\varepsilon)$ and the integrand calculated in the node of a mesh without a hole taking into consideration the function $f(\varepsilon) = -\pi\varepsilon^2$. The nodal coordinates coincide with the center of the hole (see Fig. 5). Therefore, the quotient is

$$\frac{\frac{1}{2\pi\varepsilon}\int_{\partial B_\varepsilon^0}\left(\frac{1}{2}\mathbf{S}_\varepsilon\cdot\mathbf{E}_\varepsilon\right)d\partial B_\varepsilon^0}{\frac{1}{2}\mathbf{S}\cdot\mathbf{E}}. \tag{67}$$

The result is illustrated in the plots of Fig. 8. Based on them, an asymptotic behavior of (67) can be seen when ε decreases for all the load values $\mathbf{t}_0$. The value of the constant C tends to be less and greater than 3 when the magnitude of the load $\mathbf{t}_0$ increases, respectively, for traction and compression. The numerical asymptotic analysis allows finding only an approximated expression of the topological derivative for the vectorial problem with geometric nonlinearity.

However, it is necessary to analyze the behavior of the constant C with relation to the variation of the strain energy density at the node under which the topological derivative is calculated. A larger variation of the nodal strain energy density W when compared to the changes in the constant C for each traction load value $\mathbf{t}_0$ can be observed in Tables 2, 3, 4, and 5. Therefore, the topological derivative for the problem

Table 2 Analysis of the variation of the constant C for the first traction load case for the problem of geometric nonlinearity

$\mathbf{t}_0$	W	C
12.50	0.03186	3.00
25.00	0.12624	2.97
37.50	0.28138	2.96
150.00	4.16262	2.88
450.00	31.69029	2.75

Table 3 Analysis of the variation of the constant C for the second traction load case for the problem of geometric nonlinearity

$\mathbf{t}_0$	W	C
12.50	0.03186	3.00
25.00	0.12621	2.97
37.50	0.28133	2.96
150.00	4.16171	2.88
450.00	31.68205	2.75

under consideration can be written in the following manner:

$$D_T(\hat{\mathbf{X}}) \approx C^* \frac{1}{2}\mathbf{S}\cdot\mathbf{E}, \tag{68}$$

where C^* is a constant selected from the values obtained for C.

The same numerical procedure can be applied to the linear plane elasticity problem presented in Novotny et al. (2003) to obtain the expression for the topological derivative. According to Novotny et al. (2003), the topological derivative, except for the limit with $\varepsilon \to 0$, in plane linear elasticity problems and homogeneous Neumann boundary conditions ($\mathbf{T}_\varepsilon\mathbf{n} = \mathbf{0}$) over ∂B_ε is written in the following way:

$$d_T(\mathbf{u}_\varepsilon) = -\frac{1}{f'(\varepsilon)}\int_{\partial B_\varepsilon}\left(\frac{1}{2}\mathbf{T}_\varepsilon\cdot\nabla\mathbf{u}_\varepsilon^S\right)d\partial B_\varepsilon\ . \tag{69}$$

Analogously to the nonlinear case, Fig. 9 shows straight lines that cross the origin. It can be concluded that the integrand is a constant in relation to ε and the function $f(\varepsilon) = -\pi\varepsilon^2$ can be used. Therefore,

$$D_T(\hat{\mathbf{x}}) = \lim_{\varepsilon\to 0} d_T(\mathbf{u}_\varepsilon) = C\frac{1}{2}\mathbf{T}\cdot\nabla\mathbf{u}^S.$$

Going through the same procedure applied to the nonlinear case, the constant C for the linear case can be obtained via a numerical procedure, as illustrated in the plots of Figs. 9 and 10. This results in the value of $C = 3$, which is in accordance with the analytical

Table 4 Analysis of the variation of the constant C for the third traction load case for the problem of geometric nonlinearity

$\mathbf{t}_0$	W	C
12.50	0.04534	3.00
25.00	0.18005	2.99
37.50	0.40227	2.98
150.00	6.06545	2.86
450.00	47.85283	2.70

Table 5 Analysis of the variation of the constant C for the fourth traction load case for the problem of geometric nonlinearity

$\mathbf{t}_0$	W	C
12.50	0.12159	2.99
25.00	0.47907	2.97
37.50	1.06224	2.94
150.00	15.14929	2.80
450.00	109.83755	2.61

results obtained in Novotny et al. (2003) through an asymptotic analysis

$$D_T(\hat{\mathbf{x}}) = \frac{3}{2}\mathbf{T}\cdot\nabla\mathbf{u}^S.$$

Therefore, for the special case where $\nu = 1/3$ for plane stress problems and $\nu = 1/4$ for plane strain problems, it was possible to recover the exact expression of the topological derivative by means of the numerical asymptotic analysis, as it can be seen from the plots of Fig. 10. However, it is relevant to observe that, for the nonlinear problem being considered, it is not possible to recover the exact expression of the topological derivative. Unlike the linear problem, the value of the constant C changes as the value of the applied load is altered, as can be seen in Fig. 8.

Note that the plots of both Figs. 8 and 10, that represent the asymptotic behavior of (63) and (69), respectively, under the four load cases, undergo a variation in their values when $\varepsilon = 0.01$ $\left(\frac{1}{\varepsilon} = 100\right)$. Exceptions are the plots of Figs. 8c and 10c, which represent the asymptotic behavior of (63) and (69), respectively, for the third load case. Such variation is due to the distortion of the elements that are near to the boundary of the hole

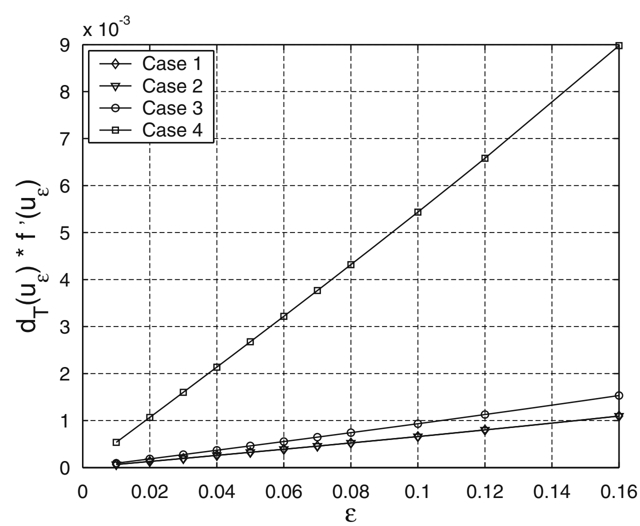

Fig. 9 Asymptotic behavior of $d_T(\mathbf{u}_\varepsilon)\ f'(\varepsilon)$ with relation to the radius ε in the plane linear elasticity problem

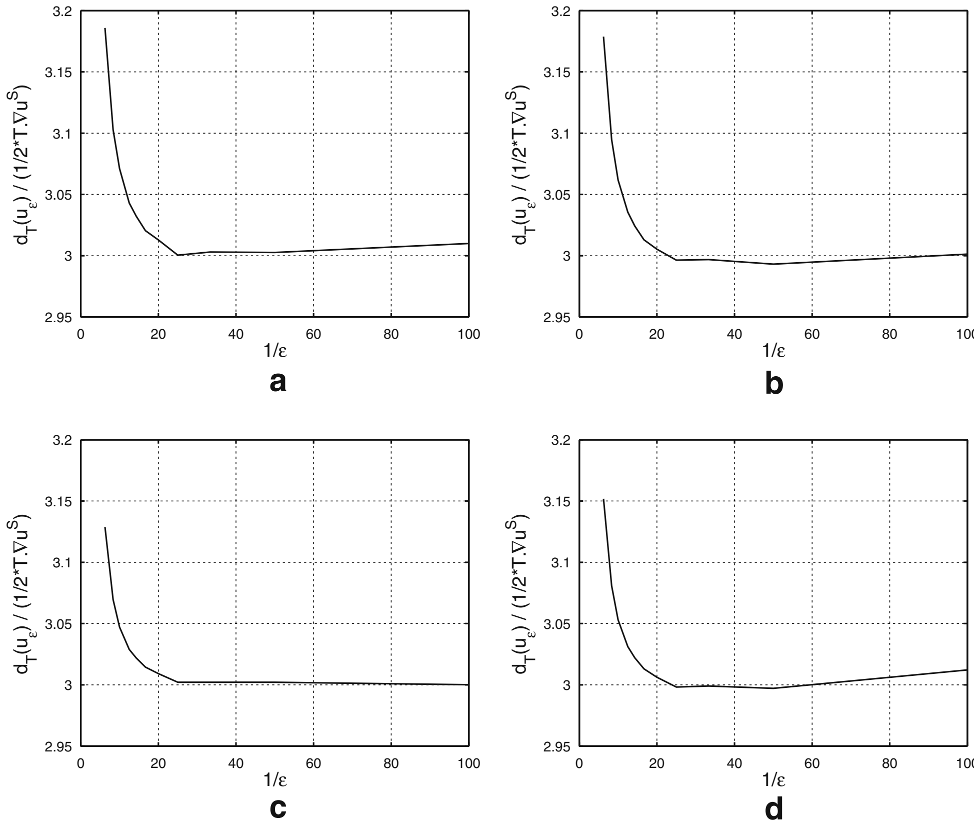

Fig. 10 Asymptotic behavior of the quotient $\frac{d_T(\mathbf{u}_\varepsilon)}{\frac{1}{2}\mathbf{T}\cdot\nabla\mathbf{u}^S}$ with relation to the radius ε for the linear plane elasticity problem. **a** First load case. **b** Second load case. **c** Third load case. **d** Fourth load case

for the first, second, and fourth load cases. On the other hand, the third load case does not distort the elements remarkably. Therefore, it does not present the variation of the other load cases.

7 Topological optimization algorithm

The topological derivative gives the sensitivity of a certain functional to the creation of small holes in the problem definition domain. It can also be used as the descending direction in a topological optimization process (Céa et al. 1998; Garreau et al. 2001; Eschenauer and Olhoff 2001). Therefore, a topological optimization algorithm that makes use of the topological derivative must obey a certain procedure for the creation of holes in the domain under study. Besides that, an additional restriction of the type

$$\int_\Omega d\Omega \leq \bar{V}, \tag{70}$$

where $\bar{V}$ is the minimum domain volume or area, is considered to avoid the algorithm leading to the trivial solution of the problem, that is $meas\,(\Omega) = 0$. The restriction given by (70) is not relaxed in the Lagrangian function (23). It is used as a stop criterion in the optimization process. In the present work, the iterative process is based on the following algorithm (Novotny et al. 2003):

Consider a sequence of domains $\{\Omega^j\}$, where j is the j-th iteration. Therefore,

1. Supply the initial domain Ω and the stop criterion, where $\bar{V}$ is the desired final area or volume and V_r the area or volume to be removed in each iteration.
2. While the stop criterion is not satisfied, do:
   (a) Solve problems (35) and (36) via FEM.
   (b) Calculate $D_T\left(\hat{\mathbf{x}}_k\right)^j$ for all nodes $\hat{\mathbf{x}}_k$ in the finite element mesh.
   (c) Create the holes at the points $\hat{\mathbf{x}}_k$ of the mesh where the values of the topological derivatives assume the minimum value till it reaches the area or volume V_r to be removed by iteration.
   (d) Define the new domain Ω^{j+1}.
   (e) Do $j = j + 1$ and return to the beginning of step 2.
3. Point where it is expected to obtain the final satisfactory topology.

The same procedure suggested in Novotny et al. (2003) was used in the creation of the holes in item c of the algorithm. Instead of adopting the point $\hat{\mathbf{x}}_k$

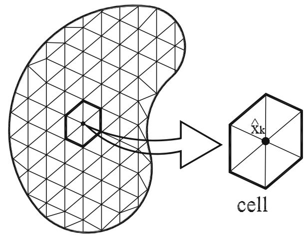

Fig. 11 Procedure for the generation of holes in the mesh

as being the barycenter of the k-th mesh element, usually known as the hard kill method (Céa et al.1998; Garreau et al. 2001), the point $\hat{\mathbf{x}}_k$ is the k-th mesh nodal point. The nodal values of the topological derivatives are obtained through a process of global smoothing of the stress and strain fields as proposed by Hinton and Campbell (1973). Therefore, the elements to be removed are those that belong to a certain cell in the mesh or the composition of all elements that share the mesh node, as illustrated in Fig. 11. In this way, according to Novotny et al. (2003), numerical instabilities are avoided and the saw tooth appearance in the final domain is minimized.

Because the algorithm for the topological optimization of linear problems differs only in the calculation of the analysis, the effective value of the constant C^* becomes of little practical interest because the topological derivative will be calculated for all the nodes in the mesh, and the holes will be created where the topological derivative assumes the least values.

8 Results

This section considers the topological optimization of large deformation plane problems. The structural component is characterized by a domain $\Omega \in \Re^2$.

8.1 Cantilever beam

In this example, the aim is to obtain the topology that minimizes the total potential energy functional of a cantilever beam model with large displacement and small strain. Consider the rectangular domain Ω with dimensions $L = 50$ mm and clamped at the left side in the regions indicated by $a = 5$ mm and submitted to a concentrated load $F = 7,500$ N, as illustrated in Fig. 12a. The finite element mesh of $11,014$ linear elements illustrated in Fig. 12b was used. Young modulus is $E = 210 \times 10^3$ N/mm^2 and Poisson coefficient $\nu = 1/4$. The final area $\bar{V}$ adopted was $\bar{V} = 0.32V_0$ and the percentage of the area to be removed in each iteration was 2%.

The final topology was attained after 56 iterations and is shown in Fig. 12c. A maximum displacement of -10.96 mm at the point of load application can be observed, which corresponds approximately to 22% of the domain height. However, the value of the strain energy density W maintains within a reasonable level. It reaches the maximum value of 35 N mm only near the clamped and load application regions and is smaller than 5.0 N mm in several regions of the domain, as can be seen in Fig. 13a. The plot of Fig. 13b illustrates the decaying of the total potential energy functional as a function of the number of iterations.

8.2 Clamped-clamped beam

In this example, a clamped-clamped beam under plane stress state is considered. The geometry is defined by the initial domain Ω of dimension $L = 20.0$ mm clamped at both side edges and submitted to a concentrated load in the middle of the span of $F = 30.0$ N, as shown in Fig. 14a. The same example is presented in Jung and Gea (2004). The mesh of 11,014 linear elements is shown in Fig. 14b for half of the domain due to the symmetry condition. It used a Young modulus of $E = 30.0$ N/mm^2 and a Poisson coefficient of $\nu = 1/3$. As the stop criterion, the final area is

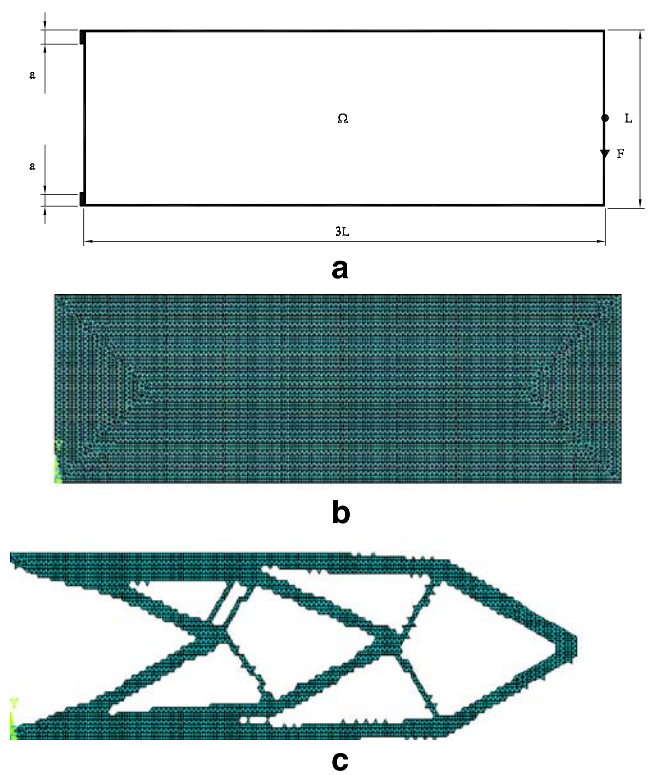

Fig. 12 Cantilever beam. **a** Model. **b** Initial mesh with 11,014 linear elements. **c** Final topology at $j = 56$

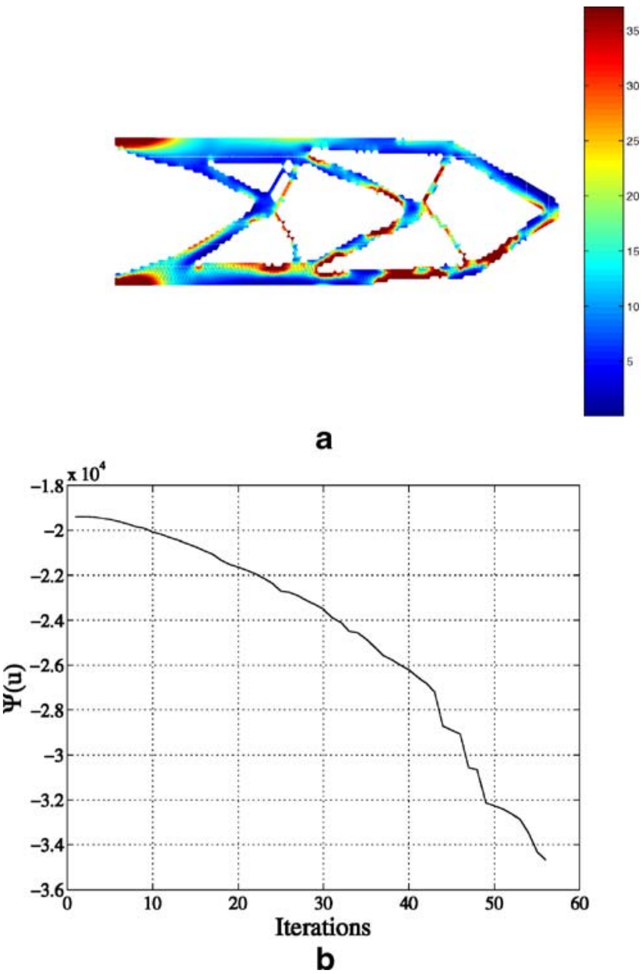

Fig. 13 Cantilever beam. **a** Energy density at iteration $j = 56$. **b** Total potential energy × iteration

$\bar{V} = 0.20V_0$ and the percentage of the area to be removed at each iteration is 2%.

The final topology was attained after 64 iterations and is shown in Fig. 14c. A maximum displacement of −4.38 mm at the point of load application can be observed, which corresponds approximately to 22% of the domain height. The value of the deformation energy density W is maintained between 0.02 and 0.20 N mm, where the largest value is in the regions where the boundary conditions are applied. Figure 14e illustrates the total potential energy functional as a function of the number of iterations.

Figure 15 illustrates the result obtained in Jung and Gea (2004) through the SIMP method for the external work density functional. The similarity between the results can be seen, except for the fact that, in the present work, the symmetry of the problem was used.

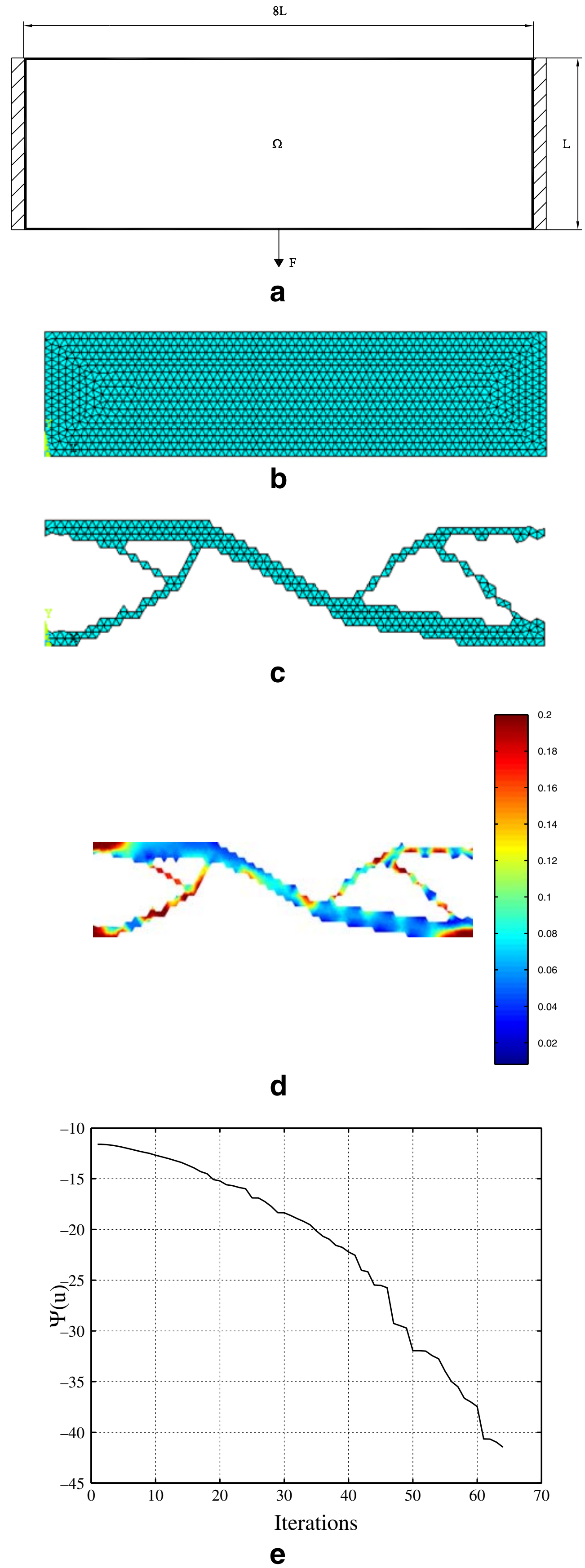

Fig. 14 Clamped-clamped beam. **a** Model. **b** Initial mesh of 11,014 linear elements. **c** Final topology at $j = 64$. **d** Energy density at iteration $j = 64$. **e** Total potential energy × iteration

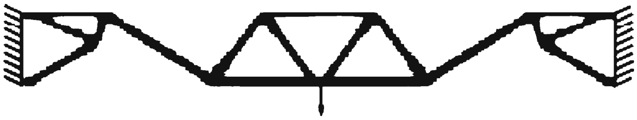

Fig. 15 Final model of the clamped beam subjected to geometric nonlinearity as given in Jung and Gea (2004)

9 Conclusions

This paper presented the application of the TSA to large deformation problems modeled using the total Lagrangian formulation. The analytical expression for the topological derivative was obtained. Due to the considered nonlinear problem and the limit presented in this expression, it cannot be calculated analytically. An approximated expression was obtained using a numerical asymptotic analysis for four different load conditions. The constant C changed for traction and compression loads but had a small range of variation. The same numerical procedure was used for the linear elasticity problem, and the analytical value for C was obtained.

A heuristic topological optimization algorithm was applied to two planar problems. For the second example, the results are similar to those obtained in the literature for the SIMP method. Based on the obtained results, the TSA may also be applied to nonlinear structural problems. The main disadvantage of the technique is the lacking of a formal minimization problem as presented in the SIMP method.

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