FROM SHAPE VARIATION TO TOPOLOGY CHANGES IN CONSTRAINED MINIMIZATION: A VELOCITY METHOD BASED CONCEPT

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Abstract. The ability of velocity methods to describe changes of topology by creating defects like holes is investigated. For the shape optimization energy-type objective functions are considered, which depend on the geometry by means of state variables. The state system is represented by abstract, quadratic, constrained minimization problems stated over domains with defects. The velocity method provides the shape derivative of the objective function due to finite variations of a defect. Sufficient conditions are derived which allow us to pass the shape derivative to the limit with respect to diminishing defect, thus, to obtain the "topological derivative" of the objective function due to a topology change. An illustrative example is presented for a circular hole bored at the tip of a crack.

1. Introduction

A rigorous description of topological changes plays a crucial role in structure optimization [1, 6, 10, 23, 30]. Our specific interest concerns the topology changes produced by creating holes, cuts, cracks and alike; for techniques and applications in the optimization context see [2, 8, 13, 34]. While the engineering and numerical applications are rather extensive, the difficulty of analysis of state systems when changing their topological properties is connected with the singular character of the problem. In order to treat the latter, singular perturbation techniques are available, however, mostly for linear partial differential equations

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(PDEs) with homogeneous coefficients; see [16, 28]. For semilinear problems see [15, 32].

On the other hand, velocity based regular perturbations are well known as a very powerful tool meeting shape optimization goals, which is well established for variational problems. We refer to [35, 7] for the foundation of velocity methods, and to [12, 21, 18, 19, 26] for the specific applications to constrained minimization problems. Moreover, level-set (implicit surface) methods can be naturally incorporated into the velocity context as described in [11, 14, 27] and other works. In the present paper, we discuss concepts adapting the velocity method to topological sensitivity analysis.

We start with a description of admissible geometries. For this purpose, let $\Omega \in \mathbb{R}^d$, $d \in \mathbb{N}$, be a domain, and x_0 a trial point in Ω. Moreover, we fix a bounded measurable set D in $\mathbb{R}^d$, associated to a generic defect, of Hausdorff dimension $m \in \mathbb{N}$, $m \leq d$, such that $0 \in D$. For $r \in \mathbb{R}_+$ we introduce the perturbed set

$$D(r) := \{y \in \mathbb{R}^d : \quad r^{-1}(y - x_0) \in D\}. \tag{D}$$

Since $x_0 \in \Omega$, there exists $R > 0$ sufficiently small such that $D(R) \subset \Omega$. Therefore, for all $r \in (0, R]$ we have $D(r) \subset \Omega$, and it is possible to define the domain with finite defect as $\Omega(r) := \Omega \setminus \overline{D(r)}$. Further, we refer to such r as the "size" of the defect. As $r \to 0$, $D(r)$ reduces to the point x_0. The limit domain $\Omega(0) = \Omega \setminus \{x_0\}$ exists (with infinitesimal defect), and it has a "continuous" topology in comparison with $\Omega(r)$ for $r > 0$. In this sense we claim that the change of topology occurs when $r \to 0$.

Since x_0 corresponding to $r = 0$ is excluded from the limit domain $\Omega(0)$, we complete the set of parameters $r \in (0, R]$ to $[0, R]$ with the limit from above $r \to 0^+$. In fact, the limit from below $r \to 0^-$ is not defined in the geometric model. We take care of these features through all of our subsequent constructions.

On every fixed domain $\Omega(r)$ with defect $D(r)$ of the size $r \in [0, R]$ we look for a state variable (scalar or vector valued) $u^r(x)$, $x \in \Omega(r)$, associated to a solution of a partial differential equation (PDE). More generally, we refer to variational solutions of associated minimization problems. Here, we consider abstract objective functionals

$$\Pi : \ H(\Omega(r)) \mapsto \mathbb{R}, \quad u \mapsto \Pi(u; \Omega(r))$$

and constrained minimization problems of the type

$$\text{minimize}\, \Pi(u; \Omega(r)) \quad \text{over}\, u \in H(\Omega(r)) \quad \text{subject to}\, u \in K(\Omega(r)). \tag{CMP}$$

Constraints are reflected by the admissible sets $K(\Omega(r))$ in vector spaces $H(\Omega(r))$ for $r \in [0, R]$. If there exists a solution $u^r \in K(\Omega(r))$ of (CMP), the associated optimal value functional is defined by $P(r) := \Pi(u^r; \Omega(r))$ with

$$(DF) \qquad P: \ [0, R] \mapsto \mathbb{R}, \quad r \mapsto \Pi(u^r; \Omega(r)).$$

We call P in (DF) a "defect function" since it serves to qualify the defects. Indeed, while $P(r)$ with $r > 0$ corresponds to the geometries having finite defects $D(r)$, the reference value of $P(0)$ belongs to the continuous geometry of Ω, *i.e.*, with the point x_0 removed only. Therefore, the increment $\Delta P := P(r) - P(0)$ compares the geometries pertinent to the two different topological situations. If $\Delta P \geq 0$, *i.e.*, $P(0) \leq P(r)$, then the optimal objective prefers the continuous geometry; otherwise, if $\Delta P < 0$, then a change of topology by creating a finite defect at x_0 is suggested. For topology optimization of Ω as well as for the identification of a defect in the domain, one needs to examine all trial points $x_0 \in \Omega$.

Generally, ΔP admits a discontinuity or oscillations as $r \to 0$. Thus, it can be ill-defined. In this paper we restrict ourselves to well posed cases and look for continuous functions $P \in C([0, R])$ satisfying an asymptotic expansion

$$(AE)$$
$$P(r) - P(0) = f(r)\, DP(x_0) + o(f(r)), \quad \text{with } \tfrac{O(f(r))}{f(r)} \to 0 \text{ as } f(r) \to 0,$$

written with respect to a strictly monotonically increasing function $f(r)$ with $f(0) = 0$. We refer to the first asymptotic term in (AE) as a "topological derivative", since $DP(x_0)$ describes exactly the sign of ΔP as $r \to 0$. Moreover, $DP(x_0)$ yields a quantitative measure for creating a defect at x_0. The order of $f(r)$ of the asymptotic expansion (AE) may depend on the underlying application; see, *e.g.*, (67) and (70) in Section 5 for examples of $f(r)$. Here, based on known results in mechanics, we consider differentiable functions P implying $f(r) = r$ only. Hence, we have the first-order asymptotic expansion

$$(AE1) \qquad P(r) - P(0) = rP'(0) + o(r), \quad \tfrac{o(r)}{r} \to 0 \text{ as } r \to 0,$$

where

$$(DD) \qquad P'(0) := \lim_{r \to 0} \frac{1}{r}\big(P(r) - P(0)\big)$$

is of order r. It yields $DP(x_0) = P'(0)$ in (AE).

The expansion in $(AE1)$ is available for a rather general class of variational problems related to elliptic PDEs [16, 28]. Note that $P'(0) = 0$ in case of $u^0 \in K(\Omega(0))$ solves (CMP) at $r = 0$ and enjoys extra smoothness (*i.e.*, exceeding the variational smoothness); see, *e.g.*, [34]. If $P'(0) = 0$, then $DP(x_0)$ is identified with the next term in the asymptotic expansion $(AE1)$. This results in (AE) with $f(r) = o(r)$. On the other hand, $P'(0) \neq 0$ for solutions u^0 in a-priori non-smooth domains Ω containing cracks and alike; see [3, 19, 20]. Even for smooth domains Ω, the assumption of extra smoothness of u^0 fails when singular data are involved like point sources, or δ-functions as adopted in the theory of fundamental solutions. For this reason we generalize the notion of a topological derivative to the first order asymptotic term in $(AE1)$ in the spirit of the method of singular perturbations [28, 29]. In this paper we provide a mathematical tool which is suitable for the calculation of $P'(0)$ and which allows us to conclude whether $P'(0) = 0$ or not.

From the point of view of perturbation theory, the principal difficulty of the sensitivity analysis of the defect function $P(r)$ as $r \to 0$ lies in the fact that it is related to singular perturbations. In order to explain the latter, observe that the definition of defects in (D) yields the flow (with respect to r) $y = x_0 + \frac{r}{R}(x - x_0) \in D(r)$ for $x \in D(R)$, which solves the dynamical system

$$(DS) \qquad \frac{dy}{dr} = \frac{y - x_0}{r} \quad \text{for } r \in (0, R], \quad y = x \text{ at } r = R.$$

The associated velocity of the defect transport is $r^{-1}(y - x_0)$. Obviously, it becomes singular at $r = 0$ which corresponds to a change of topology. We note that homeomorphic maps can be established between $\Omega(r)$ for $r > 0$ and $\Omega(0)$ as $r = 0$, but diffeomorphic properties fail. The latter, however, are essential for obtaining sensitivities. This is the reason why the asymptotic expansion based on singular perturbations in the topological context differs from sensitivities coming from shape variations, which are based on regular perturbations with smooth velocities.

We note that from $r = 0$ to $r > 0$ it is assumed that the topology of the underlying geometry changes, whence from $r > 0$ to $r + s > 0$, with $s \neq 0$, only changes of the shape of the geometry do occur. This structure is utilized to derived $(AE1)$ by the following strategy: Due to the local character of the geometric singularity at $r = 0$, we start with the shape sensitivity analysis at $r > 0$. From the *shape derivative*

$$(SD) \qquad P'(r) := \lim_{s \to 0} \frac{1}{s}\big(P(r + s) - P(r)\big) \quad \text{for } r > 0,$$

under proper assumptions we derive a weak form of $(AE1)$ given by

$$(AE1') \qquad P(r) - P(0) = \int_0^r P'(\tau)\, d\tau.$$

This results in an alternative representation of (DD) as

$$(DD') \qquad P'(0) = \lim_{r \to 0} \frac{1}{r} \int_0^r P'(\tau)\, d\tau,$$

which has to be calculated from the shape derivative (SD). This approach is justified for the specific problem of the kinking of a crack in [20]. A related concept known in the literature on topological sensitivity is based on the assertion $\lim_{r\to 0} P'(r) = P'(0)$, which is shown in [31] for smooth optimal value functions.

Motivated by applications in mechanics, in this paper we rely on quadratic objective functionals Π for (CMP), which are associated to the energy. We start in Section 2 with a velocity based kinematic description of the motion of geometric objects with defects. While finite movements serve for the sake of shape sensitivities, infinitesimal movements belong to topological changes. In Section 3 we derive the shape derivative (SD). In Section 4 we discuss sufficient conditions allowing us to pass to the limit in (DD'). Finally, in Section 5 we present an illustrative example of the topology change when a circular hole occurs at the tip of a crack.

2. Movement of geometries with defects within implicit surfaces

In this section we derive a kinematic description of the motion of geometric objects with defects for the further use in sensitivity analysis of geometry dependent problems.

For "time" (a kinematic parameter) $t \in \mathbb{R}$ we consider an evolution of sets Ω_t in $\mathbb{R}^d$ and refer these sets to an initial set Ω_0 at $t = 0$. The reference set Ω_0 is supposed to contain the finite defect $D(R)$, *i.e.*, $\Omega_0 \subset \mathbb{R}^d \setminus \overline{D(R)}$. The evolving sets are $\Omega_t \subset \mathbb{R}^d \setminus \overline{D(r)}$. In view of Section 1 we relate t to the defect size r by the relation

$$(1) \qquad |t| = -\ln(r/R) \quad \text{for } r \in (0, R],$$

or, more generally, in the sense of relations specified in (35) below. The notation of Ω_t generalizes the geometric construction $\Omega(r) := \Omega \setminus \overline{D(r)}$ in Section 1 when varying the external boundary $\partial\Omega$ with t and allowing multiple defects. Conversely, to specify the geometry, we can identify $\Omega_0 = \Omega(R)$ and $\Omega_t = \Omega(r)$.

The substitution of $t = -\ln(r/R)$ from (1) into (DS) yields the dynamic (autonomous) system with respect to $t \geq 0$

$$\frac{dy}{dt} = -(y - x_0) \quad \text{for } t > 0, \quad y = x \text{ at } t = 0. \tag{2}$$

The benefit of the substitution (1) is that the corresponding velocity of the defect transport $\mathcal{V}(y) = -(y - x_0)$ is non-singular. Note that we can use similarly the negative parameters $t = \ln(r/R)$. In Section 4 we proceed with the limit case of $|t| \to \infty$ which corresponds to $r \to 0$ when the defect $D(r)$ diminishes.

Let a time-independent kinematic velocity

$$V = (V_1, \dots, V_d)^{\mathrm{T}} \in W^{1,\infty}_{loc}(\mathbb{R}^d)^d \tag{3}$$

be given. We require that

$$V(x) = \mathcal{V}(x) \quad \text{for } x \in D(R).$$

This condition guarantees the transport of defects $D(r)$ subject to (2). In other words, we consider V as a proper extension of $\mathcal{V}$ from $D(R)$ to $\mathbb{R}^d$. For example, setting $V = \mathcal{V}\chi$ with a smooth cut-off function χ supported in Ω such that $\chi(x) = 1$ for $x \in D(R)$ is a proper extension. In this case, $\Omega_0 = \Omega \setminus \overline{D(R)}$, and $V = \mathcal{V}\chi$ yields $\Omega_t = \Omega(r)$.

Let an open, connected, bounded set (domain) Ω_0 be given by the implicit surface $\rho_0 \in W^{1,\infty}_{loc}(\mathbb{R}^d)$ as

$$\begin{aligned} &\Omega_0 = \{x = (x_1, \dots, x_d)^{\mathrm{T}} \in \mathbb{R}^d : \ \rho_0(x) > 0\}, \\ &\mathbb{R}^d \setminus \overline{\Omega}_0 = \{x \in \mathbb{R}^d : \ \rho_0(x) < 0\}, \quad \partial\Omega_0 = \{x \in \mathbb{R}^d : \ \rho_0(x) = 0\}. \end{aligned} \tag{4}$$

The sets Ω_t evolving with respect to t are represented by implicit surfaces:

$$\begin{aligned} &\Omega_t = \{y = (y_1, \dots, y_d)^{\mathrm{T}} \in \mathbb{R}^d : \ \rho(t, y) > 0\}, \\ &\mathbb{R}^d \setminus \overline{\Omega}_t = \{y \in \mathbb{R}^d : \ \rho(t, y) < 0\}, \quad \partial\Omega_t = \{y \in \mathbb{R}^d : \ \rho(t, y) = 0\}. \end{aligned} \tag{5}$$

In order to determine ρ in (5), the velocity method is utilized as specified below. In fact, for the velocity V given in (3) we require that $\rho(t, y)$ satisfies the linear transport equation

$$\frac{\partial \rho}{\partial t} + V^{\mathrm{T}} \nabla \rho = 0 \quad \text{for } t \neq 0, \quad \rho = \rho_0 \quad \text{at } t = 0. \tag{6}$$

The characteristics $y = \Phi_t(x)$ of (6) imply the autonomous system

$$\frac{d}{dt}\Phi_t = V(\Phi_t) \quad \text{for } t \neq 0, \quad \Phi_0 = x. \tag{7}$$

From the classical results of [7, 35] we infer the following lemma on the solvability of (6) and (7).

Lemma 1. *For arbitrary finite interval $\Delta_T = (0, T)$ as $t > 0$, or $\Delta_T = (-T, 0)$ as $t < 0$ with $0 < T < \infty$, there exists a unique solution of* (6) *given by*

$$\rho(t, y) = \rho_0 \circ \Phi_{-t}(y) \in W^{1,\infty}_{loc}(\Delta_T \times \mathbb{R}^d). \tag{8}$$

The backward characteristics Φ_{-t} imply a solution of (7) *corresponding to $-t$:*

$$\frac{d}{dt}\Phi_{-t} = -V(\Phi_{-t}) \quad \text{for}\, t \neq 0, \quad \Phi_0 = y. \tag{9}$$

The unique solutions of (7) *and* (9) *exist, respectively,*

$$\Phi_t, \Phi_{-t} \in C^1(\overline{\Delta}_T; W^{1,\infty}_{loc}(\mathbb{R}^d))^d, \tag{10}$$

and both functions are inverse to each other in the sense that

$$y = \Phi_t \circ \Phi_{-t}(y), \quad x = \Phi_{-t} \circ \Phi_t(x). \tag{11}$$

For the detailed derivation of Lemma 1 and its specific application to cracks see [19, 26, 27].

Note that the additional spatial smoothness $\Phi_t, \Phi_{-t} \in C^1(\overline{\Delta}_T; W^{k,\infty}_{loc}(\mathbb{R}^d))^d$ in (10) is provided by $V \in W^{k,\infty}_{loc}(\mathbb{R}^d)^d$ for arbitrary $k \in \mathbb{N}$.

In our context, Lemma 1 implies a diffeomorphism between the sets in (4) and (5) for $t \in \overline{\Delta}_T$ in the sense that

$$\begin{aligned} \Phi_t :\ \Omega_0 \mapsto \Omega_t, \quad x \mapsto \Phi_t(x) = y; \\ \Phi_{-t} :\ \Omega_t \mapsto \Omega_0, \quad y \mapsto \Phi_{-t}(y) = x. \end{aligned} \tag{12}$$

The initial condition at $t = 0$ can be shifted to $\tau = 0$ due to the semi-group property:

$$\Phi_{t+\tau} \circ \Phi_{-t}(y) = \Phi_\tau(y) \quad \text{for } \tau \in \mathbb{R}. \tag{13}$$

Indeed, from (7) we infer for every fixed τ that

$$\frac{d}{dt}\Phi_{t+\tau} = \frac{d}{d(t+\tau)}\Phi_{t+\tau} = V(\Phi_{t+\tau}), \quad \text{and } \Phi_{t+\tau}|_{\tau=0} = \Phi_t.$$

Hence, $\Phi_{t+\tau}(x) = \Phi_\tau \circ \Phi_t(x)$ together with (11) imply (13).

Using (12) and (13), from Lemma 1 we arrive at the following consequence.

Lemma 2. *For arbitrarily fixed $T > 0$ and $t \in \overline{\Delta}_T$, the coordinate transformations*

$$\begin{aligned} \Phi_\tau :\ \Omega_t \mapsto \Omega_{t+\tau}, \quad y \mapsto \Phi_\tau(y) = z; \\ \Phi_{-\tau} :\ \Omega_{t+\tau} \mapsto \Omega_t, \quad z \mapsto \Phi_{-\tau}(z) = y \end{aligned} \tag{14}$$

form a diffeomorphism with respect to τ such that $t + \tau \in \overline{\Delta}_T$.

For illustration we present the following example.

Example 1. Let $\Omega \in \mathbb{R}^d$ be a domain with a boundary $\partial\Omega$ and $\Gamma_D \subset \partial\Omega$ with $|\Gamma_D| > 0$, where $|\Gamma_D|$ denotes the measure of Γ_D. Suppose that the finite defect $D(R) \subset \Omega$ introduced in Section 1 is a domain, or, $D(R)$ is a manifold. We consider the reference domain $\Omega_0 = \Omega \setminus \overline{D(R)}$ $(= \Omega(R))$. Further, let a velocity V be given such that it satisfies (3), the boundary condition $V = 0$ at Γ_D, and $V(x) = -(x - x_0)$ for $x \in D(R)$. Then domains Ω_t evolving in $t > 0$ are determined from (5) by the implicit surface $\rho(t, \cdot\,)$ solving the transport equation (6) for this velocity V. For $x \in D(R)$ the characteristics $\Phi_t(x)$ of (6) satisfy the Cauchy problem

$$\frac{d}{dt}\Phi_t = -(\Phi_t - x_0) \quad \text{for } t > 0, \quad \Phi_0 = x.$$

Its solution is given by $\Phi_t = x_0 + (x - x_0)e^{-t}$. Consequently, from (D) we infer that the evolving sets Ω_t contain defects $D(r)$ of the size $r = Re^{-t}$ (see (1)). For $\tau > -t$, $t > 0$, we can rewrite $\Phi_{t+\tau} = x_0 + (\Phi_t - x_0)e^{-\tau}$ for $\Phi_t \in D(r)$ (compare with (13)).

Note that taking the reference domain as $\Omega_0 = \Omega \setminus \bigcup_{i=1}^N \overline{D(R_i)}$ with N finite defects $D(R_i) \subset \Omega$ of the size $R_i > 0$ given at points $x_0^i \in \Omega$ for $i = 1, \dots, N$ we arrive at a multi-defect problem, which can be treated similarly as above.

3. Shape derivative of quadratic geometry-dependent functionals

In this section, we employ the diffeomorphic maps (14) for shape sensitivity analysis of abstract constrained minimization problems.

For all $t \in \mathbb{R}$, let $K(\Omega_t)$ be a convex cone in the Hilbert space $H(\Omega_t)$ defined over the domain Ω_t, and let $H(\Omega_t)^\star$ stand for the dual space. We invoke the following assumption.

Assumption 1. *The mapping* (14) *is bijective between* $H(\Omega_t)$ *and* $H(\Omega_{t+\tau})$*, and between* $K(\Omega_t)$ *and* $K(\Omega_{t+\tau})$ *for* $t \in \overline{\Delta}_T$ *and* τ *such that* $t + \tau \in \overline{\Delta}_T$ *in the following sense:*

(15a)
$$u \in H(\Omega_t) \;\Rightarrow\; u \circ \Phi_{-\tau} \in H(\Omega_{t+\tau}), \quad v \in H(\Omega_{t+\tau}) \;\Rightarrow\; v \circ \Phi_\tau \in H(\Omega_t);$$

(15b)
$$u \in K(\Omega_t) \;\Rightarrow\; u \circ \Phi_{-\tau} \in K(\Omega_{t+\tau}), \quad v \in K(\Omega_{t+\tau}) \;\Rightarrow\; v \circ \Phi_\tau \in K(\Omega_t).$$

These assumptions are needed to derive the shape derivative in Theorem 1 below. While the bijection in (15a) is provided by Lemma 2 and a sufficient regularity of the involved transformations, the bijection in (15b) can be limiting in Assumption 1. In this context we note that, for concrete problems, the shape derivative exists under assumptions weaker than (15b). In fact, the bijection between primal cones K can be replaced with the bijection property for dual cones as suggested in [25]. Alternatively, if from $v \in K(\Omega_{t+\tau})$ it follows that $v \circ \Phi_\tau \in K_\tau(\Omega_t)$ with $K_\tau(\Omega_t) \neq K(\Omega_t)$, then the convergence $K_\tau(\Omega_t) \to K(\Omega_t)$ as $\tau \to 0$ in the Mosco sense can be helpful; see the related topic in [33]. When the bijection between $K(\Omega_t)$ and $K(\Omega_{t+\tau})$ fails, then an extra term determined by the type of constraints in K appears in formula (25) in Theorem 1.

In what follows we confine ourselves to the quadratic functionals $\Pi : H(\Omega_t) \mapsto \mathbb{R}$ defined by

$$\Pi(u; \Omega_t) := \left\langle \frac{1}{2} Au - F, u \right\rangle_{\Omega_t} \quad \text{for } u \in H(\Omega_t) \tag{16}$$

with the duality pairing $\langle \,\cdot\,, \,\cdot\, \rangle_{\Omega_t}$ between $H(\Omega_t)^\star$ and $H(\Omega_t)$. We assume that $A : H(\Omega_t) \mapsto H(\Omega_t)^\star$ for all $t \in \mathbb{R}$ is a linear, symmetric, everywhere defined operator, which is bounded and uniformly positive definite, *i.e.*,

$$c_0 \|u\|^2_{H(\Omega_t)} \leq \langle Au, u \rangle_{\Omega_t} \leq C_0 \|u\|^2_{H(\Omega_t)} \quad \text{for } u \in H(\Omega_t)$$

with $0 < c_0 \leq C_0 < \infty$ independent of t. The right-hand side $F \in L$ is given, where the space L satisfies

$$H(\Omega_t) \overset{\mathrm{u}}{\hookrightarrow} L = L^\star \overset{\mathrm{u}}{\hookrightarrow} H(\Omega_t)^\star,$$

and $\overset{\mathrm{u}}{\hookrightarrow}$ stands for the uniformly continuous embedding with respect to $t \in \mathbb{R}$. Note that according to (16), $v \mapsto \Pi(v)$ is determined also over $H(\Omega_{t+\tau})$ at the time $t + \tau$:

$$\Pi(v; \Omega_{t+\tau}) = \left\langle \frac{1}{2} Av - F, v \right\rangle_{\Omega_{t+\tau}} \quad \text{for } v \in H(\Omega_{t+\tau}). \tag{17}$$

After the application of the coordinate transformation (14) to (17) we get the functional with transformed operators $J(A \circ \Phi_\tau)$ and $J(F \circ \Phi_\tau)$, where $J := J(\Phi_\tau)$ is the Jacobian. The transformed functional is defined well over $v \circ \Phi_\tau \in H(\Omega_t)$ according to (15a) in Assumption 1, and we denote it by

$$[\Pi \circ \Phi_\tau](u; \Omega_t) := \left\langle \frac{1}{2} J\big(A \circ \Phi_\tau\big) u - J\big(F \circ \Phi_\tau\big), u \right\rangle_{\Omega_t} \in \mathbb{R} \tag{18}$$

for $u \in H(\Omega_t)$. This construction is illustrated in the example below.

For the sensitivity analysis of the transformed functional we need the following assumption.

Assumption 2. *The transformed functional* (18) *admits the following expansion with respect to small* $|\tau|$*:*

$$[\Pi \circ \Phi_\tau](u; \Omega_t) = \Pi(u; \Omega_t) + \tau \Pi^1(u, u; \Omega_t) + \mathrm{Res}_\tau(u), \tag{19a}$$

$$|\mathrm{Res}_\tau(u)| \leq a(\tau)\big(\|u\|^2_{H(\Omega_t)} + b\big), \quad 0 \leq a(\tau) = o(|\tau|), \tag{19b}$$

where $a(\,\cdot\,)$ *and* $b \geq 0$ *are independent of* Ω_t*. The first asymptotic term is given by*

$$\Pi^1(u, v; \Omega_t) := \Big\langle \frac{1}{2} A^1 u - F^1, v \Big\rangle_{\Omega_t} \quad \textit{for } u, v \in H(\Omega_t) \tag{20}$$

with a linear, symmetric, everywhere defined, bounded operator $A^1 : H(\Omega_t) \mapsto H(\Omega_t)^\star$ *for all* $t \in \mathbb{R}$*, and* $F^1 \in L$*. Note that* Π^1 *in* (20) *is not symmetric in* u *and* v *in the latter linear term.*

We illustrate the construction by means of the scalar-valued Laplace operator.

Example 2. We continue the geometric description of Example 1 and set

$$A := -\Delta, \quad H(\Omega_t) := W^{1,2}(\Omega_t), \quad L := L^2_{loc}(\mathbb{R}^d),$$
$$K(\Omega_t) := \{u \in W^{1,2}(\Omega_t) : u = 0 \text{ on } \Gamma_D,\ u \geq 0 \text{ on } \partial\Omega_t \setminus \Gamma_D\},$$

with the functional in (16) given by

$$\Pi(u; \Omega_t) = \int_{\Omega_t} \Big(\frac{1}{2}|\nabla u|^2 - F u\Big)\, dy \quad \text{for } u \in W^{1,2}(\Omega_t).$$

The notation in the definition of K implies that the traces of u are well-defined on $\partial\Omega_t$. Moreover, we assume that the Poincare–Friedrichs inequality provides a strict positive definiteness of the Laplace operator in $W^{1,2}(\Omega_0)$, hence in all spaces $W^{1,2}(\Omega_t)$. We further assume that $F \in L \cap C^1_{loc}(\mathbb{R}^d)$.

Assumption 1 holds true for this example. In fact, the bijection property in (15a) is satisfied due to (10). Indeed, the norm $\|u \circ \Phi_{-\tau}\|^2_{W^{1,2}(\Omega_{t+\tau})}$ after the transformation $z = \Phi_\tau(y)$ yields

$$\int_{\Omega_{t+\tau}} \big\{|u \circ \Phi_{-\tau}|^2 + |\nabla(u \circ \Phi_{-\tau})|^2\big\}\, dz = \int_{\Omega_t} \Big\{|u|^2 + \Big|\Big(\frac{\partial \Phi_{-\tau}}{\partial y}\Big)^{\mathrm{T}} \nabla u\Big|^2\Big\} \Big|\det \frac{\partial \Phi_\tau}{\partial y}\Big|\, dy.$$

Hence, the norm estimation $\|u \circ \Phi_{-\tau}\|_{W^{1,2}(\Omega_{t+\tau})} \leq \mathrm{c}\|u\|_{W^{1,2}(\Omega_t)}$ follows, and similarly $\|v \circ \Phi_\tau\|_{W^{1,2}(\Omega_t)} \leq \mathrm{c}\|v\|_{W^{1,2}(\Omega_{t+\tau})}$ for some $\mathrm{c} > 0$ independent of τ. The bijection in (15b) is provided by the condition $V = 0$ at

Γ_D since the Dirichlet boundary Γ_D remains fixed during the evolution of Ω_t with such a velocity V.

Next we justify Assumption 2. Applying the coordinate transformation $z = \Phi_\tau(y)$ to the perturbed functional

$$\Pi(v;\Omega_{t+\tau}) = \int_{\Omega_{t+\tau}} \Big(\frac{1}{2}|\nabla v|^2 - Fv\Big)\,dz \quad \text{for } v \in W^{1,2}(\Omega_{t+\tau})$$

we obtain the transformed functional

$$[\Pi\circ\Phi_\tau](u;\Omega_t) = \int_{\Omega_t} \Big\{\frac{1}{2}(\nabla u)^{\mathrm{T}}\frac{\partial \Phi_{-\tau}}{\partial y}\Big(\frac{\partial \Phi_{-\tau}}{\partial y}\Big)^{\mathrm{T}}\nabla u - \big(F\circ\Phi_\tau\big)u\Big\}\Big|\det\frac{\partial \Phi_\tau}{\partial y}\Big|\,dy$$

with $u \in W^{1,2}(\Omega_t)$. From (7), (10) in Lemma 1, and for small $|\tau|$ we derive the expansions

$$\Phi_{\pm\tau}(y) = y \pm \tau V(y) + \mathrm{Res}_\tau(y), \quad \|\mathrm{Res}_\tau(y)\| = o(|\tau|) \quad \text{in } W^{1,\infty}_{loc}(\mathbb{R}^d)^d,$$

$$\frac{\partial \Phi_{\pm\tau}}{\partial y} = I \pm \tau\frac{\partial V(y)}{\partial y} + \mathrm{Res}_\tau(y), \quad \|\mathrm{Res}_\tau(y)\| = o(|\tau|) \quad \text{in } L^{\infty}_{loc}(\mathbb{R}^d)^{d\times d},$$

$$\det\frac{\partial \Phi_\tau}{\partial y} = 1 + \tau \operatorname{div} V(y) + \mathrm{Res}_\tau(y), \quad \|\mathrm{Res}_\tau(y)\| = o(|\tau|) \quad \text{in } L^{\infty}_{loc}(\mathbb{R}^d),$$

where I stands for the identity matrix. Moreover, the assumed smoothness of F provides the Taylor series $F\circ\Phi_\tau = F + \tau\, V^{\mathrm{T}}\nabla F + \mathrm{Res}_\tau(\nabla F)$ with $|\mathrm{Res}_\tau(\nabla F)| = o(|\tau|)$. Substituting these expansions into the integral over Ω_t we obtain

$$\begin{aligned}
&[\Pi\circ\Phi_\tau](u;\Omega_t) = \int_{\Omega_t} \Big\{\frac{1}{2}(\nabla u)^{\mathrm{T}}\Big(I - \tau\frac{\partial V}{\partial y} - \tau\frac{\partial V}{\partial y}^{\mathrm{T}}\Big)\nabla u \\
&- \big(F + \tau\, V^{\mathrm{T}}\nabla F\big)u\Big\}\big(1 + \tau \operatorname{div} V\big)\,dy + \mathrm{Res}_\tau(u), \\
&|\mathrm{Res}_\tau(u)| \le a(\tau)\big(\|u\|^2_{W^{1,2}(\Omega_t)} + \|\nabla F\|^2_{C(\mathbb{R}^d)^d}\big), \quad 0 \le a(\tau) = o(|\tau|),
\end{aligned}$$

which leads to the asymptotic formula (19), where the first asymptotic term

(21)

$$\Pi^1(u,v;\Omega_t) = \int_{\Omega_t} \Big\{\frac{1}{2}(\nabla u)^{\mathrm{T}}\Big(\operatorname{div}(V)I - \frac{\partial V}{\partial y} - \frac{\partial V}{\partial y}^{\mathrm{T}}\Big)\nabla v - \operatorname{div}(VF)v\Big\}\,dy$$

for $u, v \in W^{1,2}(\Omega_t)$

is well known, *e.g.*, see [35]. Thus, the assumptions are true for this example.

We emphasize that this technique is suitable also for vector-valued problems and elliptic operators A with non-homogeneous coefficients; see [24, 26].

Next we investigate constrained minimization problems of the type

$$\text{minimize } \Pi(u;\Omega_t) \quad \text{over } u \in H(\Omega_t) \quad \text{subject to } u \in K(\Omega_t). \tag{22}$$

Due to the Dirichlet principle and the Lax–Milgram theorem, there exists a unique solution $u^t \in K(\Omega_t)$ of (22). By first order optimality, (22) is equivalent to the variational inequality:

$$u^t \in K(\Omega_t), \quad \langle Au^t - F, u - u^t\rangle_{\Omega_t} \geq 0 \quad \text{for all } u \in K(\Omega_t). \tag{23}$$

Our aim is to analyze the optimal value function

$$t \mapsto \Pi(u^t;\Omega_t):\ \Delta_T \mapsto \mathbb{R}, \tag{24}$$

where u^t is the unique solution of (22). For fixed $0 < T < \infty$, (24) represents variation of the shape, and further we relate it to topology changes when $T \to \infty$.

Theorem 1. *Under Assumption 1 and Assumption 2, the optimal value function* (24) *is continuously differentiable with the shape derivative*

$$\frac{d}{dt}\Pi(u^t;\Omega_t) := \lim_{\tau\to 0} \frac{\Pi(u^{t+\tau};\Omega_{t+\tau}) - \Pi(u^t;\Omega_t)}{\tau} = \Pi^1(u^t, u^t;\Omega_t). \tag{25}$$

Proof. For the proof of the assertion we proceed as follows: For fixed $t \in \Delta_T$, we start with establishing the strong convergence of the solutions $u^{t+\tau}\circ\Phi_\tau \to u^t$ as $\tau \to 0$. Based on the convergence we find the limit inferior and the limit superior in (25), which occur to be equal, thus yielding the desired derivative.

We consider the solution $u^{t+\tau} \in K(\Omega_{t+\tau})$ of the perturbed problem (22) such that

$$\Pi(u^{t+\tau};\Omega_{t+\tau}) \leq \Pi(v;\Omega_{t+\tau}) \quad \text{for all } v \in K(\Omega_{t+\tau}). \tag{26}$$

Applying the coordinate transformation $z = \Phi_\tau(y)$ to (26), from (15b) and (18) it follows that $u^{t+\tau}\circ\Phi_\tau \in K(\Omega_t)$ satisfies

$$[\Pi\circ\Phi_\tau](u^{t+\tau}\circ\Phi_\tau;\Omega_t) \leq [\Pi\circ\Phi_\tau](u;\Omega_t) \quad \text{for all } u \in K(\Omega_t). \tag{27}$$

Using $u = u^t$ in (27) results in the estimate

$$\|u^{t+\tau}\circ\Phi_\tau\|_{H(\Omega_t)} \leq c_1 + c_2\|u^t\|_{H(\Omega_t)} + O(|\tau|),$$

which is uniform for small $|\tau| \leq \delta$. Here we used (19). Hence, there exists a weakly convergent subsequence of $u^{t+\tau}\circ\Phi_\tau$, which converges to u^t as $\tau \to 0$ due to the weak lower semi-continuity of convex quadratic functionals. In view of (19), estimation of the difference of the solutions yields

$$\frac{c_0}{2}\|u^{t+\tau}\circ\Phi_\tau - u^t\|^2_{H(\Omega_t)} \le \frac{1}{2}\big\langle A(u^{t+\tau}\circ\Phi_\tau - u^t), u^{t+\tau}\circ\Phi_\tau - u^t\big\rangle_{\Omega_t}$$
$$\le \Pi(u^{t+\tau}\circ\Phi_\tau;\Omega_t) - \Pi(u^t;\Omega_t) = [\Pi\circ\Phi_\tau](u^{t+\tau}\circ\Phi_\tau;\Omega_t) - \Pi(u^t;\Omega_t) + O(|\tau|)$$
$$\le [\Pi\circ\Phi_\tau](u^t;\Omega_t) - \Pi(u^t;\Omega_t) + O(|\tau|) = O(|\tau|),$$

which implies the strong convergence

$$u^{t+\tau}\circ\Phi_\tau \to u^t \quad \text{in } H(\Omega_t) \quad \text{as } \tau\to 0. \tag{28}$$

Applying Assumption 2 and using (27) we estimate the numerator in (25) from above by

$$\Pi(u^{t+\tau};\Omega_{t+\tau}) - \Pi(u^t;\Omega_t) = [\Pi\circ\Phi_\tau](u^{t+\tau}\circ\Phi_\tau;\Omega_t) - \Pi(u^t;\Omega_t)$$
$$\le [\Pi\circ\Phi_\tau](u^t;\Omega_t) - \Pi(u^t;\Omega_t) = \tau\Pi^1(u^t,u^t;\Omega_t) + \mathrm{Res}_\tau(u^t), \quad \mathrm{Res}_\tau(u^t) = o(|\tau|).$$

On the other hand, from (22) one finds the following estimate from below:

$$[\Pi\circ\Phi_\tau](u^{t+\tau}\circ\Phi_\tau;\Omega_t) - \Pi(u^t;\Omega_t) \ge [\Pi\circ\Phi_\tau](u^{t+\tau}\circ\Phi_\tau;\Omega_t) - \Pi(u^{t+\tau}\circ\Phi_\tau;\Omega_t)$$
$$= \tau\Pi^1(u^{t+\tau}\circ\Phi_\tau, u^{t+\tau}\circ\Phi_\tau;\Omega_t) + \mathrm{Res}_\tau(u^{t+\tau}\circ\Phi_\tau), \quad \mathrm{Res}_\tau(u^{t+\tau}\circ\Phi_\tau) = o(|\tau|).$$

For $\tau\to 0$ due to (28) we arrive at the limit in (25). $\square$

The following corollary addresses the special case of identical transformations which will be useful below.

Corollary 1. *If the mapping Φ_τ in* (14) *transforms Ω_t into itself,* i.e.,

$$\Omega_{t+\tau} \equiv \Omega_t \quad \textit{for small } |\tau|, \tag{29}$$

then under Assumption 1 and Assumption 2 it holds that

$$\Pi^1(u^t,u^t;\Omega_t) = 0. \tag{30}$$

Proof. Let $\Omega_t\circ\Phi_{\pm\tau} = \Omega_t$. Applying the transformation Φ_τ to (22), due to Assumption 1 we conclude that $u^t\circ\Phi_\tau \in K(\Omega_t)$ satisfies

$$[\Pi\circ\Phi_\tau](u^t\circ\Phi_\tau;\Omega_t) \le [\Pi\circ\Phi_\tau](u;\Omega_t) \quad \text{for all } u\in K(\Omega_t). \tag{31}$$

Using Assumption 2, in the spirit of the proof of Theorem 1 we derive that

$$u^t\circ\Phi_\tau \to u^t \quad \text{strongly in } H(\Omega_t) \quad \text{as } \tau\to 0. \tag{32}$$

From (19) and (22) we infer that

$$\begin{aligned}\Pi(u^t;\Omega_t) &= [\Pi\circ\Phi_\tau](u^t\circ\Phi_\tau;\Omega_t)\\ &= \Pi(u^t\circ\Phi_\tau;\Omega_t)+\tau\,\Pi^1(u^t\circ\Phi_\tau,u^t\circ\Phi_\tau;\Omega_t)+o(|\tau|)\\ &\geq \Pi(u^t;\Omega_t)+\tau\,\Pi^1(u^t\circ\Phi_\tau,u^t\circ\Phi_\tau;\Omega_t)+o(|\tau|).\end{aligned}$$

Hence, $\Pi^1(u^t\circ\Phi_\tau,u^t\circ\Phi_\tau;\Omega_t)+\frac{o(|\tau|)}{\tau}\leq 0$, and, for $\tau\to 0$, due to (32) we obtain $\Pi^1(u^t,u^t;\Omega_t)\leq 0$. Conversely, using (31) and (19) we get

$$\begin{aligned}\Pi(u^t;\Omega_t) = [\Pi\circ\Phi_\tau](u^t\circ\Phi_\tau;\Omega_t) &\leq [\Pi\circ\Phi_\tau](u^t;\Omega_t)\\ &= \Pi(u^t;\Omega_t)+\tau\,\Pi^1(u^t,u^t;\Omega_t)+o(|\tau|).\end{aligned}$$

Therefore, $\Pi^1(u^t,u^t;\Omega_t)+\frac{o(|\tau|)}{\tau}\geq 0$, and the passage $\tau\to 0$ yields in the limit $\Pi^1(u^t,u^t;\Omega_t)\geq 0$. Hence, (30) follows. □

For a differentiability analysis of optimal value functions for abstract optimization problems we refer to [5]. It is interesting to note that formula (25) does not include any variation of u^t with respect to changing domains (such as material or shape derivatives; see [35] for the definition of these two concepts). This nice feature is due to the fact that the functionals in the objective (24) and in the state problem (22) coincide. In the general case, shape derivatives of objective functions include variations of the state variables with respect to geometry changes. Further investigations on this theme can be found in [17]. In contrast to the situation above, we will see that expansions of the solution u^t (the state variable) play a crucial role for the topological changes considered in the next section.

4. Derivative of objective functionals when topology changes

Our aim is to apply the results of the previous section to describe topological changes. In particular, we consider diminishing defects in a continuous domain. These features can be described as the limit case when $t\to\infty$ (we rely on $t>0$).

In view of Section 1, the geometric construction of $\Omega_t=\Omega(r)$ with $\Omega(r):=\Omega\setminus\overline{D(r)}$ provides that for $t\to\infty$ (equivalently, as $r\to 0$) the limit domain $\Omega_\infty=\Omega\setminus\{x_0\}$ exists. Motivated by this construction we suggest the following generalization.

Assumption 3. *There exists a limit domain $\Omega_\infty\subset\mathbb{R}^d$ such that*

$$\Omega_\infty=\bigcup_{t=0}^{\infty}\Omega_t. \tag{33}$$

$$D_t := \Omega_\infty \setminus \Omega_t, \quad \mathrm{meas}(D_t) \to 0 \quad \textit{as}\, t \to \infty. \tag{34}$$

In the specific case of $\Omega_t = \Omega(r)$ Assumption 3 is satisfied, and we associate D_t in (34) with the diminishing defect $D(r)$ of the size r due to relation (1). We consider (1) as a particular case of general connection between the kinematic parameter t and the defect size r given by

$$\begin{aligned} &t = \psi(r) : [0, R] \mapsto \overline{\mathbb{R}}_+ \text{ strictly monotonically decreasing,} \\ &\psi \in C^1_{loc}((0, R]), \quad \psi(R) = 0, \quad \psi(r) \to \infty \quad \text{as } r \to 0. \end{aligned} \tag{35}$$

Note that $\psi'(r) < 0$ and $\psi'(r) \to -\infty$ as $r \to 0$ in (35). In this notation (1) reads $\psi(r) = -\ln(r/R)$ and $\psi'(r) = -1/r$.

Based on Assumption 3 and using notation (35) we can state the constrained minimization problem (22) in $\Omega_{\psi(0)} = \Omega_\infty$:

$$\text{minimize } \Pi(u; \Omega_{\psi(0)}) \quad \text{over } u \in H(\Omega_{\psi(0)}) \quad \text{subject to } u \in K(\Omega_{\psi(0)}). \tag{36}$$

Problem (36) admits a unique solution $u^{\psi(0)} \in K(\Omega_{\psi(0)})$ in the Hilbert space $H(\Omega_{\psi(0)})$. Restating the optimal value function (24) in terms of r given in (35), we get

$$P : \ [0, R] \mapsto \mathbb{R}, \quad r \mapsto \Pi(u^{\psi(r)}; \Omega_{\psi(r)}), \tag{37}$$

where $u^{\psi(r)} = u^t$ is the solution of (22). After substitution of (35) into (7) we arrive at the system

$$\frac{d}{dr}\Phi_{\psi(r)} = \psi'(r) V(\Phi_{\psi(r)}) \quad \text{for } r \in (0, R), \quad \Phi_{\psi(R)} = x. \tag{38}$$

Hence, applying the chain rule to (25) and using the velocity $\psi'(r)V$ due to (38), from Theorem 1 we conclude the following result.

Theorem 2. *The objective function* (37) *is continuously differentiable in* $(0, R]$ *with the derivative*

$$P'(r) = \psi'(r)\, \Pi^1(u^{\psi(r)}, u^{\psi(r)}; \Omega_{\psi(r)}) \quad \textit{for}\, r > 0. \tag{39}$$

Formula (39) becomes singular at $r = 0$ due to the presence of $\psi'(r)$. Below, however, we shall find that $\Pi^1(u^{\psi(r)}, u^{\psi(r)}; \Omega_{\psi(r)})$ balances this singularity of $\psi'(r)$ as $r \to 0$. In Lemma 3 we establish an auxiliary result concerning the limit value of $\Pi^1(u^{\psi(0)}, u^{\psi(0)}; \Omega_{\psi(0)})$ as $r \to 0$. Indeed, for any τ the mapping Φ_τ transforms $\Omega_{\psi(0)}$ into itself due to (33). Therefore, from Theorem 1 and Corollary 1 the next result follows immediately.

Lemma 3. *If Assumptions 1 and 2 are satisfied in the limit domain* $\Omega_{\psi(0)}$, i.e.,

(15a): $$u \in H(\Omega_{\psi(0)}) \;\Rightarrow\; u \circ \Phi_\tau \in H(\Omega_{\psi(0)}),$$

(15b): $$u \in K(\Omega_{\psi(0)}) \;\Rightarrow\; u \circ \Phi_\tau \in K(\Omega_{\psi(0)}) \quad \textit{for all } \tau \in \mathbb{R};$$

(19a): $$[\Pi \circ \Phi_\tau](u; \Omega_{\psi(0)}) = \Pi(u; \Omega_{\psi(0)}) + \tau \Pi^1(u, u; \Omega_{\psi(0)}) + \mathrm{Res}_\tau(u),$$

(19b): $$|\mathrm{Res}_\tau(u)| \le a(\tau)\big(\|u\|^2_{H(\Omega_{\psi(0)})} + b\big), \quad 0 \le a(\tau) = o(|\tau|), \quad b \ge 0,$$

then it holds that

$$\Pi^1(u^{\psi(0)}, u^{\psi(0)}; \Omega_{\psi(0)}) = 0. \tag{40}$$

Now Theorem 2 and Lemma 3 allow us to use (39) in order to describe topological changes in $\Omega_\infty = \Omega_{\psi(0)}$. Therefore, our aim is to study the limit

$$\lim_{r \to 0} \frac{\Pi(u^{\psi(r)}; \Omega_{\psi(r)}) - \Pi(u^{\psi(0)}; \Omega_{\psi(0)})}{r} := P'(0). \tag{41}$$

Based on Theorem 2 we represent (41) equivalently as

(42)
$$P'(0) = \lim_{r \to 0} \frac{1}{r} \int_0^r P'(\tau)\, d\tau = \lim_{r \to 0} \frac{1}{r} \int_0^r \psi'(\tau)\, \Pi^1(u^{\psi(\tau)}, u^{\psi(\tau)}; \Omega_{\psi(\tau)})\, d\tau.$$

As we observe from Lemma 3, the formal passage to the limit in (42) is indefinite because of $\Pi^1(u^{\psi(r)}, u^{\psi(r)}; \Omega_{\psi(r)}) \to 0$ and $\psi'(r) \to -\infty$ as $r \to 0$. To clarify this indefiniteness, an expansion of the state variable $u^{\psi(r)}$ with respect to $r \to 0$ is needed. Moreover, a local expansion is sufficient when the shape derivative is determined locally in $\Omega_{\psi(r)}$. Such a localization of shape derivatives on subsets was established in the structure theorems in [9, 35]. As another example, we mention the well-known path-independent Cherepanov–Rice integral of energy representing the shape derivative due to crack propagation; see (55) in the example below. These considerations motivate the following assumption.

Assumption 4. *For all* $r \in (0, R]$ *there exist subdomains* $\mathcal{O}_r \subset \Omega_{\psi(r)}$ *such that*

$$\Pi^1(u^{\psi(r)}, u^{\psi(r)}; \Omega_{\psi(r)}) = \Pi^1(u^{\psi(r)}, u^{\psi(r)}; \mathcal{O}_r), \tag{43a}$$

$$\Pi^1(u^{\psi(0)}, u^{\psi(0)}; \Omega_{\psi(0)}) = \Pi^1(u^{\psi(0)}, u^{\psi(0)}; \mathcal{O}_r). \tag{43b}$$

Based on Assumption 4, in the following proposition we state sufficient conditions on the solution to obtain the limit in (42).

Proposition 1. *If the conditions*

$$\text{(44a)}\quad \text{(i)}\qquad \|u^{\psi(r)} - u^{\psi(0)}\|_{H(\Omega_{\psi(r)})} \to 0 \quad \text{as } r \to 0,$$

$$\text{(44b)}\quad \text{(ii)}\qquad 0 \le -\psi'(r)\|u^{\psi(r)} - u^{\psi(0)}\|_{H(\mathcal{O}_r)} \le \text{const}$$

hold, then the mapping $r \mapsto P(r)$ *in* (37) *obeys the expansion:*

(45a)

$$P(r) = P(0) + Q(r) + O\Big(-\int_0^r \frac{d\tau}{\psi'(\tau)}\Big), \quad \textit{where } -\int_0^r \frac{d\tau}{\psi'(\tau)} = o(r),$$

$$\text{(45b)}\qquad Q(r) := \int_0^r \Pi^1\big(2u^{\psi(0)}, \psi'(\tau)(u^{\psi(\tau)} - u^{\psi(0)}); \mathcal{O}_\tau\big)\, d\tau = O(r).$$

If the mapping $r \mapsto P'(r)$ *defined in* (39) *is monotone, then the limit in* (42) *exists and it is given by*

$$\text{(46)}\qquad P'(0) = \lim_{r\to 0} r^{-1} Q(r).$$

Proof. The relations (39) and (43a) imply that

$$\text{(47)}\qquad P(r+s) = P(r) + \int_r^{r+s} \psi'(\tau)\Pi^1(u^{\psi(\tau)}, u^{\psi(\tau)}; \mathcal{O}_\tau)\, d\tau.$$

We represent $u^{\psi(\tau)} = u^{\psi(0)} + (u^{\psi(\tau)} - u^{\psi(0)})$ in (47). Applying Lemma 3 and (43b) yields the following decomposition for small τ

$$\text{(48a)}\quad \begin{aligned} &\psi'(\tau)\Pi^1(u^{\psi(\tau)}, u^{\psi(\tau)}; \mathcal{O}_\tau) = \Pi^1\big(2u^{\psi(0)}, \psi'(\tau)(u^{\psi(\tau)} - u^{\psi(0)}); \mathcal{O}_\tau\big) \\ &+ \Pi^1\big(u^{\psi(\tau)} - u^{\psi(0)}, \psi'(\tau)(u^{\psi(\tau)} - u^{\psi(0)}); \mathcal{O}_\tau\big), \end{aligned}$$

$$\text{(48b)}\quad \begin{aligned} &\Pi^1\big(u^{\psi(\tau)} - u^{\psi(0)}, \psi'(\tau)(u^{\psi(\tau)} - u^{\psi(0)}); \mathcal{O}_\tau\big) = O\big(-(\psi'(\tau))^{-1}\big), \\ &\text{where } -(\psi'(\tau))^{-1} \to 0 \quad \text{as } \tau \to 0. \end{aligned}$$

Here the estimate (48b) is provided by (20) and (44b). Using (48), from (47) we obtain the expansion

$$\text{(49)}\quad \begin{aligned} &P(r+s) = P(r) + \int_r^{r+s} \Pi^1\big(2u^{\psi(0)}, \psi'(\tau)(u^{\psi(\tau)} - u^{\psi(0)}); \mathcal{O}_r\big)\, d\tau \\ &+ O\Big(-\int_0^s \frac{d\tau}{\psi'(\tau)}\Big). \end{aligned}$$

The convergence $P(r) \to P(0)$ as $r \to 0$ in (49) is ensured by the condition (44a). From (28) with $t + \tau = \psi(r+s)$ and $t = \psi(s)$, thus $\tau = r\psi'(s) + o(r)$, we infer

$$\begin{aligned} &P(r+s) = \Pi(u^{\psi(r+s)}; \Omega_{\psi(r+s)}) = [\Pi \circ \Phi_\tau](u^{\psi(r+s)} \circ \Phi_\tau; \Omega_{\psi(s)}) \\ &= \Pi(u^{\psi(r+s)} \circ \Phi_\tau; \Omega_{\psi(s)}) + O(r) \to \Pi(u^{\psi(s)}; \Omega_{\psi(s)}) = P(s) \quad \text{as } r \to 0. \end{aligned}$$

Therefore, passing $r \to 0$ in (49), applying the Lebesgue dominated convergence theorem and changing the notation of s to r yields (45).

The existence of the unique limit in (46) is not guaranteed when the sequence $P'(r)$ admits oscillations as $r \to 0$. Indeed, the uniform bound in (44b) implies that particular limits $\{Q\} = \lim_{r_n \to 0} P'(r_n)$, $|Q| < \infty$, exist on subsequences r_n only. Nevertheless, if $r \mapsto P'(r)$ is monotone, then $\lim_{r \to 0} P'(r) = P'(0)$ is unique, and it coincides with the limit in (46) with Q from (45). $\square$

We conclude Proposition 1 with remarks on the conditions in (44). Note that (44a) yields the necessary and sufficient condition for existence of $P'(0)$. The convergence in (44a) can be justified by variational methods. In contrast, to obtain the sufficient condition (44b) in the subdomain $\mathcal{O}_r$ one needs asymptotics of the solution. In practical applications, the asymptotic analysis usually utilizes Fourier series. Its justification in varying domains, however, needs a Saint–Venant principle; see the related topic in [4, 22]. In the next section we give an example illustrating the expansion of the solution which provides $P'(0)$ in Proposition 1.

5. Example: circular hole at the tip of a crack

We present an example of a topological change produced by the creation of a circular hole in a reference domain, which is non-smooth due to the presence of a crack inside. Our consideration follows the structure of Sections 2–4.

5.1. **Kinematic description.** We start with a kinematic description. In view of Section 1, let the reference domain Ω in $\mathbb{R}^2$ contain a rectilinear crack Γ_C of length $l > 0$ with one end tip located at the trial point x_0. For convenience of notation, we set the origin 0 at x_0 and associate a Cartesian coordinate system (x_1, x_2) such that $\Gamma_C = \{x : x_1 \in [-l, 0], x_2 = 0\}$. Let the boundary $\partial\Omega$ of Ω consist of a simple contour Γ (referred to as the external boundary) and the two crack faces Γ_C^+ and Γ_C^-. We assume that Γ is a Lipschitz curve.

We take the generic defect D in the form of a unit disk. For further use we denote by B_r the open disk of radius $r > 0$ centered at 0 (the trial point). There exists $R \in (0, l)$ sufficiently small such that, for all $r \in (0, R)$, the disks B_r represent defects $D(r)$ of the size r in Ω. Then the evolving domains $\Omega(r) = \Omega \setminus \overline{B(r)}$ are well-defined. Further we denote by n the unit normal vector at the boundary $\partial\Omega(r)$ consisting of Γ, ∂B_r, and $\Gamma_C^\pm \setminus B_r$.

We choose the defect velocity $\mathcal{V}(x) = -x$, for $x \in B_R$, and the kinematic velocity $V(y) := -y\chi(y)$ with a smooth cut-off function χ, with $\chi : \mathbb{R}^2 \mapsto [0,1]$ such that $\chi(y) = 1$ for $y \in B_{R/2}$, and $\chi(y) = 0$ for $y \in \mathbb{R}^2 \setminus B_R$. Introducing the kinematic parameter $t \in [0,\infty]$ by $t = \psi(r)$ with $\psi(r) := -\ln(r/R)$ yields the kinematic description of Section 2 of the evolving domains $\Omega_t = \Omega_{\psi(r)} = \Omega(r)$. In this section we rely on the unified notation $\Omega_{\psi(r)}$ for the domain with the fixed crack Γ_C and the diminishing defect (disk B_r) of size $r \in [0,R]$ at the crack tip.

5.2. **Problem formulation.** We consider the following boundary value problem stated in $\Omega_{\psi(r)}$: For all $r \in [0,R]$ find $u^{\psi(r)}$ satisfying

$$-\Delta u^{\psi(r)} = F \quad \text{in } \Omega_{\psi(r)}, \tag{50a}$$

$$u^{\psi(r)} = 0 \quad \text{on } \Gamma, \tag{50b}$$

$$\frac{\partial u^{\psi(r)}}{\partial n} = 0 \quad \text{on } \partial B_r \cup (\Gamma_C^{\pm} \setminus B_r). \tag{50c}$$

Here, $F \in C^1(\overline{\Omega})$ is given, and we assume $F = 0$ in $B_{R/2}$. For $r = 0$ (50) turns into the following problem stated in the reference domain $\Omega_{\psi(0)}$: Find $u^{\psi(0)}$ satisfying

$$-\Delta u^{\psi(0)} = F \quad \text{in } \Omega_{\psi(0)}, \tag{51a}$$

$$u^{\psi(0)} = 0 \quad \text{on } \Gamma, \tag{51b}$$

$$\frac{\partial u^{\psi(0)}}{\partial n} = 0 \quad \text{on } \Gamma_C^{\pm}. \tag{51c}$$

For the feasible set

$$K(\Omega_{\psi(r)}) := \{u \in W^{1,2}(\Omega_{\psi(r)}) : u = 0 \text{ on } \Gamma\},$$

the weak solution $u^{\psi(r)} \in K(\Omega_{\psi(r)})$ of (50) is guaranteed to exist uniquely as the minimizer of the energy functional

$$\Pi(u; \Omega_{\psi(r)}) := \int_{\Omega_{\psi(r)}} \Big(\frac{1}{2}|\nabla u|^2 - Fu\Big)\, dy \tag{52}$$

over $u \in W^{1,2}(\Omega_{\psi(r)})$ subject to $u \in K(\Omega_{\psi(r)})$.

5.3. **Shape derivative and its structure.** The optimal value (defect) function is given by

$$P:[0,R]\mapsto\mathbb{R},\quad r\mapsto \Pi(u^{\psi(r)};\Omega_{\psi(r)})=\int_{\Omega_{\psi(r)}}\Bigl(\frac{1}{2}|\nabla u^{\psi(r)}|^2-Fu^{\psi(r)}\Bigr)\,dy.$$

From Theorems 1 and Theorems 2, for $r\in(0,R)$ the existence of the limit

$$\begin{aligned}&\lim_{\tau\to 0}\frac{\Pi(u^{\psi(r+\tau)};\Omega_{\psi(r+\tau)})-\Pi(u^{\psi(r)};\Omega_{\psi(r)})}{\tau}\\ &=-\frac{1}{r}\,\Pi^1(u^{\psi(r)},u^{\psi(r)};\Omega_{\psi(r)})=:P'(r)\end{aligned}\tag{53}$$

with $-1/r=\psi'(r)$ follows. Using the calculation of Example 2, from (21) we infer that

$$\begin{aligned}&\Pi^1(u,v;\Omega_{\psi(r)})\\ &=\int_{\Omega_{\psi(r)}}\Bigl\{\frac{1}{2}(\nabla u)^{\mathrm{T}}\Bigl(\mathrm{div}(V)I-\frac{\partial V}{\partial y}-\frac{\partial V}{\partial y}^{\mathrm{T}}\Bigr)\nabla v-\mathrm{div}(VF)v\Bigr\}\,dy.\end{aligned}\tag{54}$$

Note that $V(y)=-y$ for $y\in B_\rho$, $\rho\in(0,R/2)$, in view of our construction of the velocity. This yields $\mathrm{div}(V)I-\frac{\partial V}{\partial y}-\frac{\partial V}{\partial y}^{\mathrm{T}}=0$ in B_ρ. Moreover, $F=0$ in B_ρ, and $V=0$ in $\Omega\setminus B_R$. Hence, the domain of integration in (54) reduces to the annulus $\mathcal{O}_r:=(B_R\setminus B_r)\setminus\Gamma_C$, and Assumption 4 of the structure of the shape derivative holds true in this example. Thus, we obtain

$$\begin{aligned}\Pi^1(u^{\psi(r)},u^{\psi(r)};\mathcal{O}_r)&=\int_{\mathcal{O}_r}\Bigl\{\frac{1}{2}(\nabla u^{\psi(r)})^{\mathrm{T}}\Bigl(\mathrm{div}(V)I-\frac{\partial V}{\partial y}-\frac{\partial V}{\partial y}^{\mathrm{T}}\Bigr)\nabla u^{\psi(r)}\\ &-\mathrm{div}(VF)u^{\psi(r)}\Bigr\}\,dy.\end{aligned}$$

The solution of (50) enjoys extra $W^{2,2}$-smoothness away from the crack tips. Therefore, integration by parts yields

$$\begin{aligned}\Pi^1(u^{\psi(r)},u^{\psi(r)};\mathcal{O}_r)&=\int_{\mathcal{O}_r}\bigl(\Delta u^{\psi(r)}+F\bigr)\bigl(V^{\mathrm{T}}\nabla u^{\psi(r)}\bigr)\,dy\\ &+\int_{\partial B_r}\Bigl\{\frac{1}{2}(V^{\mathrm{T}}n)|\nabla u^{\psi(r)}|^2-\bigl(V^{\mathrm{T}}\nabla u^{\psi(r)}\bigr)\bigl(n^{\mathrm{T}}\nabla u^{\psi(r)}\bigr)\Bigr\}\,dS_y.\end{aligned}$$

Using equation (50a), $n=-y/|y|$, $V=-y$ and $|y|=r$ at ∂B_r, we obtain

$$\Pi^1(u^{\psi(r)},u^{\psi(r)};\mathcal{O}_r)=r\int_{\partial B_r}\Bigl\{\frac{1}{2}|\nabla u^{\psi(r)}|^2-\Bigl(\frac{\partial u^{\psi(r)}}{\partial n}\Bigr)^2\Bigr\}\,dS_y.\tag{55}$$

In fracture mechanics, (55) is well known as the Cherepanov–Rice integral. We note that the latter term in (55) is zero due to (50c).

5.4. **Expansion of solutions.** To calculate the integral in (55) we construct a local representation of the solution $u^{\psi(r)}$ in $\mathcal{O}_r$. For this aim we follow the method of matched asymptotic expansions of [16, 28].

We introduce a polar coordinate system $\rho = |y|$, $\theta \in (-\pi, \pi)$ at 0 such that the crack faces $\Gamma_C^\pm$ correspond to $\theta = \pm\pi$. For the solution $u^{\psi(0)}$ of the reference problem (51), its local asymptotic expansion is known, and it is given by the Fourier series in $B_R \setminus \Gamma_C$ as

(56)
$$u^{\psi(0)}(y) = u^{\psi(0)}(0) + c_1\rho^{\frac{1}{2}} \sin\frac{\theta}{2} + a_1\rho\cos\theta + b_1\rho\sin\theta + U, \quad U = O(\rho^{\frac{3}{2}}).$$

The unique coefficients $c_1, a_1, b_1 \in \mathbb{R}$ in (56) can be calculated using the weight functions of the respective order. For fixed $r \in (0, R/2)$, let us denote the difference of solutions by $w^r := u^{\psi(r)} - u^{\psi(0)}$. Due to (50) and (51), the function $w^r \in K(\Omega_{\psi(r)})$ satisfies the following equations:

$$-\Delta w^r(y) = 0 \quad \text{for } y \in \Omega_{\psi(r)}, \tag{57a}$$

$$w^r(y) = 0 \quad \text{for } y \in \Gamma, \quad \frac{\partial w^r}{\partial n}(y) = 0 \quad \text{for } y \in \Gamma_C^\pm, \tag{57b}$$

$$\frac{\partial w^r}{\partial n}(y) = -\frac{\partial u^{\psi(0)}}{\partial n}(y) \quad \text{for } y \in \partial B_r. \tag{57c}$$

Rewriting (57) in the stretched variable $\xi := y/r$ and passing $|\xi| \to \infty$ we arrive at the second limit problem in the exterior domain: Find W^r satisfying

$$-\Delta W^r(\xi) = 0 \quad \text{for } \xi \in (\mathbb{R}^2 \setminus \overline{B_1}) \setminus \Gamma_\infty, \tag{58a}$$

$$\frac{\partial W^r}{\partial n}(\xi) = 0 \quad \text{for } \xi \in (\mathbb{R}^2 \setminus \overline{B_1}) \cap \Gamma_\infty^\pm, \tag{58b}$$

$$\frac{\partial W^r}{\partial n}(\xi) = -r\frac{\partial u^{\psi(0)}}{\partial n}(r\xi) \quad \text{for } \xi \in \partial B_1, \tag{58c}$$

with the semi-infinite crack $\Gamma_\infty := \{(\xi_1, \xi_2) \in \mathbb{R}^2 : \xi_1 \le 0, \xi_2 = 0\}$. From (56) we have $\int_{\partial B_1} \partial u^{\psi(0)}/\partial n \, dS_\xi = 0$ which implies the solvability condition of the exterior Neumann problem (58) in the weighted Sobolev space

$$X := \{\mu v, \nabla v \in L^2((\mathbb{R}^2 \setminus \overline{B_1}) \setminus \Gamma_\infty)\}, \quad \mu \sim \big(|\xi| \ln|\xi|\big)^{-1} \quad \text{as } |\xi| \to \infty.$$

The weight μ is due to the Poincaré inequality in exterior domains. Excluding constant values, there exists the unique solution $W^r \in X \setminus \mathbb{R}$ to (58) yielding the Fourier series in $(\mathbb{R}^2 \setminus \overline{B_1}) \setminus \Gamma_\infty$ as

(59)
$$W^r(\xi) = c_1^r |\xi|^{-\frac{1}{2}} \sin\frac{\theta}{2} + \frac{a_1^r}{|\xi|}\cos\theta + \frac{b_1^r}{|\xi|}\sin\theta + V(\xi), \quad V = O(|\xi|^{-\frac{3}{2}}).$$

Substituting expansions (56) and (59) into (58c) we determine the unknown coefficients c_1^r, a_1^r, b_1^r from the orthogonal decomposition

$$\begin{aligned}\frac{\partial W^r}{\partial n}(\xi)\Big|_{|\xi|=1} &= \frac{c_1^r}{2}\sin\frac{\theta}{2} + a_1^r\cos\theta + b_1^r \sin\theta + \frac{\partial V}{\partial n}(\xi)\Big|_{|\xi|=1} \\ = -r\frac{\partial u^{\psi(0)}}{\partial n}(r\xi)\Big|_{|\xi|=1} &= \frac{c_1}{2} r^{\frac{1}{2}} \sin\frac{\theta}{2} + a_1\cos\theta + b_1\sin\theta - r\frac{\partial U}{\partial n}(r\xi)\Big|_{|\xi|=1}.\end{aligned}$$

Henceforth, $c_1^r = r^{\frac{1}{2}} c_1$, $a_1^r = r a_1$, $b_1^r = r b_1$. Using the inverse substitution $y = r\xi$ in (59) we get in $(\mathbb{R}^2 \setminus \overline{B_r}) \setminus \Gamma_\infty$ the Fourier series

(60)
$$\begin{aligned}&W^r\Big(\frac{y}{r}\Big) = r c_1 \rho^{-\frac{1}{2}} \sin\frac{\theta}{2} + r^2 a_1 \rho^{-1}\cos\theta + r^2 b_1 \rho^{-1}\sin\theta + V^1 \\ &\text{with } V^1(y) := V(y/r) = O\Big(r^3 \rho^{-\frac{3}{2}}\Big).\end{aligned}$$

The asymptotic formulas yield the expansion $u^{\psi(r)} = u^{\psi(0)} + W^r + Q$ in $\mathcal{O}_r$, where $W^r = O(r^{\frac{1}{2}})$ in $\Omega_{\psi(r)}$ due to $W^r = O(r^{\frac{1}{2}})$ at ∂B_r. The residual $Q := w^r(y) - W^r(y/r) \in H(\Omega_{\psi(r)})$ satisfies the equations

(61a)
$$-\Delta Q(y) = 0 \quad \text{for } y \in \Omega_{\psi(r)},$$

(61b)
$$Q(y) = -W^r\Big(\frac{y}{r}\Big) \quad \text{for } y \in \Gamma, \quad \frac{\partial Q}{\partial n}(y) = 0 \quad \text{for } y \in \Gamma_C^\pm,$$

(61c)
$$\frac{\partial Q}{\partial n}(y) = 0 \quad \text{for } y \in \partial B_r.$$

Since $W^r(y/r) = O(|c_1| r + r^2)$ at Γ, from (61) we can estimate $Q = O(|c_1| r + r^2)$ in $\Omega_{\psi(r)}$. Thus, (60) results in the local asymptotic expansion of the solution $u^{\psi(r)}$ of (50) in $\mathcal{O}_r$ given by the expression

(62)
$$u^{\psi(r)} = u^{\psi(0)} + r c_1 \rho^{-\frac{1}{2}} \sin\frac{\theta}{2} + r^2 a_1 \rho^{-1}\cos\theta + r^2 b_1 \rho^{-1}\sin\theta + Q + V^1.$$

We note that the residual $Q + V^1$ does not impact the formulas of topological derivatives derived in the following section.

5.5. **Topological derivatives.** Now we are in a position to calculate the integral in (55), which we rewrite in polar coordinates as

$$\Pi^1(u^{\psi(r)}, u^{\psi(r)}; \mathcal{O}_r) = \frac{1}{2}\int_{-\pi}^{\pi} \Big\{ \Big(\frac{\partial u^{\psi(r)}}{\partial \theta}\Big)^2 - r^2 \Big(\frac{\partial u^{\psi(r)}}{\partial \rho}\Big)^2 \Big\}\Big|_{\rho=r} d\theta. \tag{63}$$

We remind that $\partial u^{\psi(r)}/\partial\rho = 0$ at $\rho = r$ according to (50c). Inserting the expansions (56) and (62) in (63), some technical calculations lead to

$$\Pi^1(u^{\psi(r)}, u^{\psi(r)}; \mathcal{O}_r) = \frac{\pi}{2}c_1^2 r + 2\pi(a_1^2+b_1^2)r^2 + O\big(|c_1|(r^{\frac{3}{2}}+r^2)+r^3\big), \tag{64}$$

with the terms of order $O\big(|c_1|(r^{\frac{3}{2}}+r^2)\big)$ due to Q in (62). By using (64), from (53) we obtain the expansion of the shape derivative

$$P'(r) = -\frac{\pi}{2}c_1^2 - 2\pi(a_1^2+b_1^2)r + O\big(|c_1|(r^{\frac{1}{2}}+r)+r^2\big). \tag{65}$$

Passing with $r \to 0$ in (65) yields the existence of the topological derivative

$$P'(0) = -\frac{\pi}{2}c_1^2. \tag{66}$$

The coefficient c_1 in (66) is uniquely defined. It characterizes the leading singularity of the reference solution $u^{\psi(0)}$ near the trial point 0, and it is called the stress intensity factor in fracture mechanics.

Now we justify the assertion of Proposition 1. Indeed, similar to (63) some manipulations yield

$$\Pi^1(2u^{\psi(0)}, \psi'(r)w^r; \mathcal{O}_r) = -\frac{1}{r}\int_{-\pi}^{\pi} \Big\{ \frac{\partial u^{\psi(0)}}{\partial \theta}\frac{\partial w^r}{\partial \theta} - r^2 \frac{\partial u^{\psi(0)}}{\partial \rho}\frac{\partial w^r}{\partial \rho} \Big\}\Big|_{\rho=r} d\theta$$
$$= -\frac{\pi}{2}c_1^2 - 8\pi c_1 b_1 r^{\frac{1}{2}} - 2\pi(a_1^2+b_1^2)r + O\big(|c_1|(r^{\frac{1}{2}}+r)+r^2\big)$$

with $\psi'(r) = -1/r$. Therefore, in the notation of (45), we have $Q(r) = -\frac{\pi}{2}c_1^2 r + O(r^{\frac{3}{2}})$, and $P'(0) = \lim_{r\to 0} Q(r)/r$ coincides with (66). We conclude that Proposition 1 becomes useful when an exact analytic expansion of shape derivatives like (64) is not available directly.

The knowledge of the exact analytic expansion (64) provides us with the following results. Using $P(r) - P(0) = \int_0^r P'(\tau)\,d\tau$, from (65) one finds the asymptotic expansion of the defect function P with respect to $r \to 0$ as

$$P(r) = P(0) - \frac{\pi}{2}c_1^2 r - \pi(a_1^2+b_1^2)r^2 + O\big(|c_1|(r^{\frac{3}{2}}+r^2)+r^3\big). \tag{67}$$

Finally, we consider the specific case when the solution of the reference problem (51) enjoys extra smoothness. Let $u^{\psi(0)} \in W^{2,2}(B_R \setminus \Gamma_C)$, which exceeds the variational $W^{1,2}$-smoothness of the solution justified by the minimization problem. In this case, $c_1 = 0$ in (56) and one obtains

$$u^{\psi(0)}(y) = u^{\psi(0)}(0) + a_1\rho\cos\theta + b_1\rho\sin\theta + O(\rho^{\frac{3}{2}}) \quad \text{in } B_R \setminus \Gamma_C.$$

Differentiating this equality and then passing with $\rho \to 0$ ensures that $(a_1, b_1)^{\mathrm{T}} = \nabla u^{\psi(0)}(0)$. Therefore, (56) turns into

$$u^{\psi(0)}(y) = u^{\psi(0)}(0) + y^\top \nabla u^{\psi(0)}(0) + O(|y|^{\frac{3}{2}}) \quad \text{in } B_R \setminus \Gamma_C, \tag{68}$$

and, similarly, (62) reads

$$u^{\psi(r)}(y) = u^{\psi(0)}(y) + \frac{r^2}{|y|^2}\big(y^\top \nabla u^{\psi(0)}(0)\big) + O\Big(r^3 |y|^{-\frac{3}{2}}\Big) \quad \text{in } \mathcal{O}_r. \tag{69}$$

If $c_1 = 0$, from (67) we infer the second order expansion

$$P(r) = P(0) - \pi r^2 |\nabla u^{\psi(0)}(0)|^2 + O(r^3). \tag{70}$$

The term $-\pi r^2 |\nabla u^{\psi(0)}(0)|^2$ in (70) implies the topological derivative presented in [31, 34].

Conclusion

Based on these findings we conclude the following. While the “topological derivative” is suitable for the description of changes of topology restricted to smooth data, our generalization of the concept within singular perturbations has a rather broad scope of generally non-smooth data subject to topological changes.

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