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Adjoint-based methods to compute higher-order topological derivatives with an application to elasticity

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Abstract

Purpose – The goal of this paper is to give a comprehensive and short review on how to compute the first- and second-order topological derivatives and potentially higher-order topological derivatives for partial differential equation (PDE) constrained shape functionals.

Design/methodology/approach – The authors employ the adjoint and averaged adjoint variable within the Lagrangian framework and compare three different adjoint-based methods to compute higher-order topological derivatives. To illustrate the methodology proposed in this paper, the authors then apply the methods to a linear elasticity model.

Findings – The authors compute the first- and second-order topological derivatives of the linear elasticity model for various shape functionals in dimension two and three using Amstutz' method, the averaged adjoint method and Delfour's method.

Originality/value – In contrast to other contributions regarding this subject, the authors not only compute the first- and second-order topological derivatives, but additionally give some insight on various methods and compare their applicability and efficiency with respect to the underlying problem formulation.

Keywords Topological derivative, Topology optimisation, Elasticity

Paper type Research paper

1. Introduction

In this paper we provide a review of techniques for the computation of the first- and secondorder topological derivatives. We compare and apply three techniques to the following model problem: Let $D \subset \mathbf{R}^d$, d = 2, 3, be a bounded and smooth domain. Let $\Gamma \subset \partial D$, $\Gamma_N := \partial D \setminus \Gamma$ and $\Gamma_m \subset \Gamma_N$ be given. The goal is it to compute the topological derivative of the cost functional

$$\mathcal{J}(\mathbf{\Omega}) = \gamma_f \int_{\mathsf{D}} f_{\mathbf{\Omega}} \cdot u_{\mathbf{\Omega}} \, dx + \gamma_g \int_{\mathsf{D}} |\nabla u_{\mathbf{\Omega}} - \nabla u_d|^2 \, dx + \gamma_m \int_{\Gamma_m} |u_{\mathbf{\Omega}} - u_m|^2 \, dS, \qquad (1.1)$$

 $\gamma_f, \gamma_g, \gamma_m \in \mathbf{R}, \gamma_g = \gamma_m = 0$ in $d = 2, u_d \in H^1(\mathsf{D}), u_m \in L_2(\Gamma_m)$ subject to a design region $\Omega \subset \mathsf{D}$ and the displacement field $u_\Omega \in H^1(\mathsf{D})^d$ satisfies $u_\Omega|_{\Gamma} = u_D$ and solves the equation of linear elasticity

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$$\int_{\mathsf{D}} \mathbf{C}_{\Omega} \boldsymbol{\epsilon}(u_{\Omega}) : \boldsymbol{\epsilon}(\varphi) \, dx = \int_{\mathsf{D}} f_{\Omega} \cdot \varphi \, dx + \int_{\Gamma_N} u_N \cdot \varphi \, dS \quad \text{for all } \varphi \in H^1_{\Gamma}(\mathsf{D})^d, \qquad (1.2)$$



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where $H_{\Gamma}^{1}(\mathsf{D})^{d} := \{\varphi \in H^{1}(\mathsf{D}) : \varphi = 0 \text{ on } \Gamma\}$ denotes the standard Sobolev space. Here, $u_{D} \in L_{2}(\Gamma), u_{N} \in L_{2}(\Gamma_{N})$ are given functions and the coefficient functions $\mathbf{C}_{\Omega}, f_{\Omega}$ are defined methods piecewise by

$$\mathbf{C}_{\Omega} = \mathbf{C}_{1}\chi_{\Omega} + \mathbf{C}_{2}\chi_{D\setminus\overline{\Omega}}, \quad f_{\Omega} = f_{1}\chi_{\Omega} + f_{2}\chi_{D\setminus\overline{\Omega}}, \tag{1.3}$$

where $\mathbf{C}_1, \mathbf{C}_2: \mathbf{R}^{d \times d} \to \mathbf{R}^{d \times d}$ are linear functions, $f_1, f_2 \in H^1(\mathsf{D})^d \cap C^2(B_\delta(x_0))^d$, $\delta > 0$ and $\epsilon(u)$ denotes the symmetrised gradient of u, that is, $\epsilon(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$. Let $x_0 \in \mathsf{D}$ be a given point and $\omega \subset \mathbf{R}^d$ a smooth open set containing the origin $0 \in \omega$.

Let $x_0 \in D$ be a given point and $\omega \subset \mathbf{R}^a$ a smooth open set containing the origin $0 \in \omega$. Moreover, denote by $\omega_{\varepsilon} := x_0 + \varepsilon \omega$, $\varepsilon > 0$ small the perturbation at x_0 by the inclusion ω . We are going to discuss the asymptotic expansion of \mathcal{J} of a singularly perturbed domain by adding the inclusion $\omega_{\varepsilon} \subset D \setminus \overline{\Omega}$ to Ω , that is, $\Omega_{\varepsilon} = \Omega \cup \omega_{\varepsilon}$ and $x_0 \in D \setminus \overline{\Omega}$. For the sake of simplicity of the presentation, we are going to consider the case $\Omega = \emptyset$. However, we note that the other scenario where $\Omega \neq \emptyset$ and $\Omega_{\varepsilon} = \Omega \setminus \omega_{\varepsilon}$ (i.e. $x_0 \in \Omega$) can be treated in a similar fashion leading only to minor changes in the presented derivations.

The topological derivative was first introduced in Eschenauer *et al.* (1994) and later mathematically justified in Sokolowski and Zochowski (1999), Garreau *et al.* (2001) with an application to linear elasticity. Follow-up works of many authors studied the asymptotic behaviour of shape functionals for various partial differential equations (PDEs). For instance, for Kirchhoff plates Amstutz and Novotny (2010), electrical impedance tomography Hintermüller and Laurain (2008), Hintermüller *et al.* (2011), Maxwell's equation Masmoudi *et al.* (2005), Stokes' equation Hassine and Masmoudi (2004) and elliptic variational inequalities Hintermüller and Laurain (2011). We also refer to the monograph Novotny and Sokolowski (2013) for more applications and references therein.

The idea of the topological derivative is to perturb the design variable with a singular perturbation and study the asymptotic behaviour of the shape functional .7. The asymptotic expansion encodes information about the optimal topology of the design region and can be used numerically either in an iterative level-set method Amstutz and Andrä (2006) or oneshot-type methods Hintermüller and Laurain (2008), Sokolowski and Zochowski (1999) to obtain an optimal topology of the design region (in the sense of stationary points). Higherorder topological derivatives are a viable means to improve the accuracy of one-shot-type methods as done in Hintermüller and Laurain (2008), Bonnet and Cornaggia (2017), Finally, let us also mention a one-shot Newton-type method as described in Chapter 10 of Novotny and Sokołowski (2019) using higher-order topological expansions. The idea is to consider minclusions (typically ball-shaped) at the same time and compute their topological expansion. This expansion is then used to solve a Newton-type equation leading to an efficient and robust way to determine inclusions (also called anomalities, inhomogeneities or obstacles) even when noise is present. An application to electrical impedance tomography can be found in Hintermüller et al. (2011), Canelas et al. (2015) and (Novotny and Sokołowski, 2019, Chap. 11). We refer to (Novotny and Sokołowski, 2019, Chap. 10) and references therein for further applications, such as inverse conductivity, electromagnetic casting and obstacle reconstruction.

Higher-order topological derivatives are less studied, but have been computed for several problems. For instance, in Hintermüller and Laurain (2008), second-order topological derivatives for an electrical impedance tomography problem are studied. In Bonnet (2018), higher-order topological derivatives in dimension two for linear elasticity using the method of Novotny *et al.* (2003) are established. In Bonnet and Cornaggia (2017), the expansion of higher-order topological derivatives for a least square misfit function for linear elasticity in dimension three exploiting a Green's function is established. In Bonnet (2018), a similar misfit function subject to a scattering problem is expanded.

The first ingredient to compute higher topological derivatives is the asymptotic behaviour of the solution of the state equation, in our concrete example this is Equation (1.2). The second ingredient is an expansion of the shape function and is mostly, although not necessary, done via the introduction of an adjoint variable. As is well known from optimal control and shape optimisation theory (see, e.g. Hinze *et al.*, 2009; Ito and Kunisch, 2008), the advantage of using an adjoint variable is the numerically efficient computation of the topological derivative. First-order topological derivatives for ball inclusions and linear problems can be computed solely from the knowledge of the state variable and the adjoint state variable; see, for example, in Sokolowski and Zochowski (1999). For higher-order topological derivatives in most cases, additional exterior partial differential equations, so-called corrector equations, have to be solved, although in some cases these can also be solved explicitly; Hintermüller and Laurain (2008).

While most papers deal with linear partial differential equations, also nonlinear partial differential equations have been studied. We refer to Iguernane *et al.* (2009), Beretta *et al.* (2017), Sturm (2020), Amstutz (2006b) for the study of first-order topological derivatives for semilinear elliptic partial differential equations. To the authors' knowledge, there is no research for higher-order topological derivatives for these equations and thus remains an open and challenging topic. Also, quasi-linear problems have been studied first in Amstutz and Bonnafé (2017) and more recently in Gangl and Sturm (2020a), Amstutz and Gangl (2019), Gangl and Sturm (2021). In particular in Gangl and Sturm (2020a), a projection trick is used to avoid the use of a fundamental solution, which is in contrast to most works on semilinear partial differential equations.

An established method to compute the topological derivative and higher derivatives is the method of Amstutz (2003). It amounts to study the asymptotic behaviour of a perturbed adjoint equation, which depends on the unperturbed state equations. It has been used in some of the papers mentioned above such as Masmoudi *et al.* (2005), Hassine and Masmoudi (2004) and also Amstutz (2006a, b), to only mention a few. The advantage of the method is that it simplifies the computation of the topological derivative compared to a direct computation of the topological derivative by expanding the cost function with Taylor's expansion.

A second method, which has been introduced in the context of shape optimisation and the computation of shape derivatives, was used in Sturm (2020) to compute topological derivatives for semilinear problems. It has been extended in Gangl and Sturm (2020a) to compute topological derivatives for quasi-linear problems. In contrast to Amstutz' method, the averaged adjoint variable also depends on the perturbed state equation, which makes the anaylsis of the asymptotic behaviour of the adjoint variable more challenging. However, the advantage is that it seems to be readily applicable to a wide range of cost functions, and also the computation of the final formula for higher-order topological derivatives is straight forward once the asymptotics of the averaged adjoint variable is known.

A third method was introduced in Delfour (2018) and uses the usual unperturbed adjoint variable. The advantage is that no analysis of a perturbed adjoint variable is required, but, as shown in Gangl and Sturm (2020a), it seems to be more difficult to apply this method to certain cost functions, such as the L_2 -tracking-type cost functions.

Finally, let us mention the method of Novotny *et al.* (2003), where a method to compute the topological derivatives is proposed as the limit of the shape derivative. This method is not always applicable, but it provides a fast method to compute also higher-order topological derivatives; see Silva *et al.* (2010).

In this paper we thoroughly study and review the first three mentioned methods and apply them to the model problem of linear elasticity introduced in (1.2). We first exam the asymptotic behaviour of (1.2) up to order two and then study the asymptotic behaviour of Amstutz' perturbed adjoint variable and the averaged adjoint variable. We then apply the three methods to compute first- and second-order topological derivatives for three types of

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cost functions, the compliance, a boundary tracking-type cost function and a tracking-type Adjoint-based cost function of the gradient.

1.1 Structure of the paper

In Section 2, we discuss three different teqhniques to compute the topological derivative. This is done by introducing the Lagrangian setting, which simplifies the notation. In Section 3, we derive the complete asymptotic analysis for a linear elasticity model including remainder estimates. The section covers both the two-dimensional and three-dimensional cases, whose analysis differs since the fundamental solution of the linear elasticity equation has a different asymptotic behaviour. In Section 4, we derive the asymptotic analysis for the adjoint and averaged adjoint variable, respectively. This is done in a similar fashion to Section 3. In Section 5, we employ the previously derived results to compute the topological derivative. That is, we apply the theoretical background derived in Section 2 to our elasticity model and a versatile cost function.

1.2 Notation

In the whole paper we denote by $W_p^1(D)$ (resp. their vector-valued counter parts by $W_p^1(D)^d$) for $1 \le p \le \infty$ standard Sobolev spaces equipped with the usual norm. The gradient of a function $\varphi \in W_p^1(D)$ (resp. $\varphi \in W_p^1(D)^d$) will be denoted $\nabla \varphi$. Directional derivatives of functions $f: U \subset \mathbf{E} \to \mathbf{R}$ at $x \in \mathbf{E}$ defined on an open subset $U \subset \mathbf{E}$ of a Banach space \mathbf{E} will be denoted by $\partial f(x)(v), x \in U, v \in \mathbf{E}$ whenever it exists. Similarly for functions $(u, v) \mapsto f(u, v) : \mathbf{E} \times \mathbf{F} \to \mathbf{R}$, we denote their partial derivative with respect to the first (resp. second) argument by $\partial_u f(x_1, x_2)(v)$ (resp. $\partial_v f(x_1, x_2)(w)$). We further define for $1 \le p \le \infty$

$$BL_p\left(\mathbf{R}^d\right)^d := \left\{\varphi \in W^1_{p,loc}(\mathsf{D})^d : \nabla \varphi \in L_p(\mathsf{D})^{d \times d}\right\}.$$

Then we define the Beppo-Levi space $\dot{BL}_p(\mathbf{R}^d)^d := BL(\mathbf{R}^d)^d / \mathbf{R}$ equipped with $\|[\varphi]\|_{\dot{BL}_p(\mathbf{R}^d)^d} := \|\nabla\varphi\|_{L_p(\mathbf{R}^d)^{d \times d}}, \varphi \in [\varphi], [\varphi] \in \dot{BL}_p(\mathbf{R}^d)^d$. Here $/\mathbf{R}$ means that we quotient out constants.

The Euclidean norm on \mathbf{R}^d will be denoted as $|\cdot|$ and the corresponding operator norm $\mathbf{R}^{d \times d}$ will be also denoted as $|\cdot|$. The Euclidean ball of radius r > 0 located at $x_0 \in \mathbf{R}^d$ will be denoted as $B_r(x_0)$. Additionally, for a domain Ω with sufficiently smooth boundary $\partial \Omega$, we denote the outer normal vector as n. The Slobodeckij seminorm $|\cdot|_{H^{\frac{1}{2}}(\Omega)}$ for $\Omega \subset \mathbf{R}^d$ is defined by

$$|u|_{H^{\frac{1}{2}}(\Omega)} := \left(\int_{\Omega} \int_{\Omega} \frac{|u(x) - u(y)|^2}{|x - y|^{d+1}} \, dx dy \right)^{\frac{1}{2}}.$$

For convenience we will later on use the abbreviated notation of the averaged integral defined as

$$\oint_{\Omega} f \, dx := \frac{1}{|\Omega|} \int_{\Omega} f \, dx,$$

for a bounded set $\Omega \subset \mathbf{R}^d$.

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2. Lagrangian techniques to compute the topological derivative

In this section we review Lagrangian techniques to compute topological derivatives. While it is well established in optimisation algorithms to compute derivatives of PDE constrained problems with the help of Lagrangians, it seems rather new to the topology optimisation community. However, we will show that actually Amustutz's method can be interpreted as a Lagrangian approach by introducing a suitable Lagrangian function and recasting his original result in terms of this Lagrangian. More recently, another Lagrangian approach was proposed in Delfour and Sturm (2016), where essentially an extra term appears when differentiating the Lagrangian function. Finally, we will review Delfour's approach of (Delfour, 2018, Thm.3.3) using only the unperturbed adjoint state variable.

2.1 Abstract setting

Let \mathcal{V}, \mathcal{W} be real Hilbert spaces. For all parameter $\varepsilon \ge 0$ small consider a function $u_{\varepsilon} \in \mathcal{V}$ solving the variational problem of the form

$$a_{\varepsilon}(u_{\varepsilon},\varphi) = f_{\varepsilon}(\varphi) \quad \text{for all } \varphi \in \mathcal{W}, \tag{2.1}$$

where a_{ε} is a bilinear form on $\mathcal{V} \times \mathcal{W}$ and f_{ε} is a linear form on \mathcal{W} , respectively. Throughout we assume that this abstract state equation admits a unique solution and that $u_{\varepsilon} - u_0 \in \mathcal{W}$ for all ε , where $u_0 \in \mathcal{V}$ denotes the unperturbed state variable satisfying

$$a_0(u_0, \varphi) = f_0(\varphi) \quad \text{for all } \varphi \in \mathcal{W},$$
(2.2)

and a_0, f_0 are the unperturbed counterparts to the bilinear form a_{ε} and linear form f_{ε} , respectively. Consider now a cost function

$$j(\varepsilon) = J_{\varepsilon}(u_{\varepsilon}) \in \mathbf{R},\tag{2.3}$$

where for all $\varepsilon \ge 0$, the functional $J_{\varepsilon} : \mathcal{V} \to \mathbf{R}$ is differentiable at u_0 . In the following sections we review methods how to obtain an asymptotic expansion of $j(\varepsilon)$ at $\varepsilon = 0$. For this purpose we introduce the Lagrangian function

$$\mathcal{L}(\varepsilon, u, v) = J_{\varepsilon}(u) + a_{\varepsilon}(u, v) - f_{\varepsilon}(v), \quad u \in \mathcal{V}, \ v \in \mathcal{W}.$$

2.2 Amstutz' method

We first review the approach of Amstutz (2003); see also (Amstutz, 2006a, Prop. 2.1). This approach has been proved to be versatile and has been applied to a number of linear and non-linear problems. For instance, in Amstutz (2006a) a linear transmission problem was examined and its first-order topological derivative was computed. In Amstutz *et al.* (2014), the topological derivative of elliptic differentiation equations with 2*m* differential operator was derived. In Amstutz (2006b), the topological derivative for a class of certain non-linear equations has been studied.

Proposition 2.1. (Amstutz, 2006a, Prop. 2.1). Assume that the following hypotheses hold.

(1) There exist numbers $\delta a^{(1)}$ and $\delta f^{(1)}$ and a function $\ell_1 : \mathbf{R}^+ \to \mathbf{R}^+$ with $\lim_{\epsilon \searrow 0} \ell_1(\epsilon) = 0$, such that

$$(a_{\varepsilon} - a_0)(u_0, p_{\varepsilon}) = \ell_1(\varepsilon)\delta a^{(1)} + o(\ell_1(\varepsilon)), \qquad (2.4)$$

$$(f_{\varepsilon} - f_0)(p_{\varepsilon}) = \ell_1(\varepsilon)\delta f^{(1)} + o(\ell_1(\varepsilon)), \qquad (2.5)$$

where $p_{\varepsilon} \in \mathcal{W}$ is the adjoint state satisfying

 $a_{\varepsilon}(\varphi, p_{\varepsilon}) = -\partial J_{\varepsilon}(u_0)(\varphi) \quad \text{for all } \varphi \in \mathcal{V}. \tag{2.6}$ methods

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(2) There exist two numbers $\delta J_1^{(1)}$ and $\delta J_2^{(1)}$, such that

$$J_{\varepsilon}(u_{\varepsilon}) = J_{\varepsilon}(u_0) + \partial J_{\varepsilon}(u_0)(u_{\varepsilon} - u_0) + \ell_1(\varepsilon) \partial J_1^{(1)} + o(\ell_1(\varepsilon)), \qquad (2.7)$$

$$J_{\varepsilon}(u_0) = J_0(u_0) + \ell_1(\varepsilon) \delta J_2^{(1)} + o(\ell_1(\varepsilon)).$$
(2.8)

Then the following expansion holds

$$j(\varepsilon) = j(0) + \ell_1(\varepsilon) \Big(\delta a - \delta f^{(1)} + \delta J_1^{(1)} + \delta J_2^{(1)} \Big) + o(\ell_1(\varepsilon)).$$
(2.9)

We will reformulate and generalise the previous result in terms of a Lagrangian function $\mathcal{L}(\varepsilon, u, v)$ and additionally state a result for the second-order derivative. Therefore, note that $p_0 \in \mathcal{W}$ denotes the unperturbed adjoint state variable satisfying

$$a_0(\varphi, p_0) = -\partial J_{\varepsilon}(u_0)(\varphi) \quad \text{for all } \varphi \in \mathcal{V}.$$
(2.10)

Proposition 2.2.

(1) Let $\ell_1 : \mathbf{R}^+ \to \mathbf{R}^+$ be a function with $\lim_{\epsilon \searrow 0} \ell_1(\epsilon) = 0$. Furthermore, assume that the limits

$$\mathcal{R}^{(1)}(u_0, p_0) := \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_\varepsilon, p_\varepsilon) - \mathcal{L}(\varepsilon, u_0, p_\varepsilon)}{\ell_1(\varepsilon)},$$
(2.11)

$$\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0) := \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_0, p_{\varepsilon}) - \mathcal{L}(0, u_0, p_{\varepsilon})}{\ell_1(\varepsilon)},$$
(2.12)

exist. Then we have the following expansion:

$$j(\varepsilon) = j(0) + \ell_1(\varepsilon) \Big(\mathcal{R}^{(1)}(u_0, p_0) + \partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0) \Big) + o(\ell_1(\varepsilon)).$$
(2.13)

In particular, $\mathcal{R}^{(1)}(u_0, p_0) + \partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0) = \delta a^{(1)} - \delta f^{(1)} + \delta J_1^{(1)} + \delta J_2^{(1)}$, where $\delta a^{(1)}$, $\delta f_1^{(1)}, \delta J_1^{(1)}, \delta J_2^{(1)}$ are as in Proposition 2.1.

(2) Let $\ell_2 : \mathbf{R}^+ \to \mathbf{R}^+$ be a function with $\lim_{\epsilon \to 0} \frac{\ell_2(\epsilon)}{\ell_1(\epsilon)} = 0$. Furthermore, assume that the assumptions under (1) hold and that the limits

$$\mathcal{R}^{(2)}(u_0, p_0) := \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_\varepsilon, p_\varepsilon) - \mathcal{L}(\varepsilon, u_0, p_\varepsilon) - \ell_1(\varepsilon) \mathcal{R}^{(1)}(u_0, p_0)}{\ell_2(\varepsilon)}, \qquad (2.14)$$

$$\partial_{\ell}^{(2)} \mathcal{L}(0, u_0, p_0) := \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_0, p_{\varepsilon}) - \mathcal{L}(0, u_0, p_{\varepsilon}) - \ell_1(\varepsilon) \partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0)}{\ell_2(\varepsilon)}, \quad (2.15)$$

exist. Then we have the following expansion

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$$egin{aligned} j(arepsilon) &= j(0) + \ell_1(arepsilon) igg(\mathcal{R}^{(1)}(u_0,p_0) + \partial_\ell^{(1)}\mathcal{L}(0,u_0,p_0)igg) + \ell_2(arepsilon) igg(\mathcal{R}^{(2)}(u_0,p_0) \ + \partial_\ell^{(2)}\mathcal{L}(0,u_0,p_0)igg) + o(\ell_2(arepsilon)). \end{aligned}$$

Proof. ad (1): Using that
$$\mathcal{L}(\varepsilon, u_{\varepsilon}, 0) = \mathcal{L}(\varepsilon, u_{\varepsilon}, p_{\varepsilon})$$
 and $\mathcal{L}(0, u_0, p_{\varepsilon}) = \mathcal{L}(0, u_0, 0)$ we get.
 $j(\varepsilon) - j(0) = \mathcal{L}(\varepsilon, u_{\varepsilon}, 0) - \mathcal{L}(0, u_0, 0)$ (2.16)

$$= \mathcal{L}(\varepsilon, u_{\varepsilon}, p_{\varepsilon}) - \mathcal{L}(\varepsilon, u_0, p_{\varepsilon})$$
(2.17)

$$+ \mathcal{L}(\varepsilon, u_0, p_{\varepsilon}) - \mathcal{L}(0, u_0, p_{\varepsilon}).$$
(2.18)

Now, the result follows by dividing by $\ell_1(\varepsilon)$ for $\varepsilon > 0$ and passing to the limit $\varepsilon \searrow 0$. ad (2): This follows the same lines as the proof of item (1) and is left to the reader.

Remark 2.3.

- (1) Checking the expansions (2.12), (2.15) in applications usually requires some regularity of the state u_0 and knowledge of the asymptotics of the adjoint state p_{ε} on a small domain of size ε .
- (2) The computation of the asymptotic expansions (2.11), (2.14) requires the study of the asymptotic behaviour of u_{ε} on the whole domain D. This often causes problems, especially in dimension two. The reader will find an application of this method in Section 5.1.

2.3 Averaged adjoint method

Another approach to compute topological derivatives was proposed in Sturm (2020) and applied to non-linear problems in Gangl and Sturm (2020a), Sturm (2020), Gangl and Sturm (2021) and used for the optimisation on surfaces in Gangl and Sturm (2020b). Recall the Lagrangian function

$$\mathcal{L}(\varepsilon, u, v) = J_{\varepsilon}(u) + a_{\varepsilon}(u, v) - f_{\varepsilon}(v), \quad u \in \mathcal{V}, \ v \in \mathcal{W}.$$
(2.19)

We henceforth assume that for all $(\varphi, q) \in \mathcal{V} \times \mathcal{W}$ and $\varepsilon \geq 0$ the function

$$s \mapsto \partial_u \mathcal{L}(\varepsilon, su_\varepsilon + (1-s)u_0, q)(\varphi) : [0,1] \to \mathbf{R}$$
 (2.20)

is continuously differentiable. With the Lagrangian we can define the averaged adjoint equation associated with state variables u_{ε} (solution of (2.1) for $\varepsilon > 0$) and u_0 (solution of (2.1) for $\varepsilon = 0$): find $q_{\varepsilon} \in \mathcal{W}$, such that

$$\int_{0}^{1} \partial_{u} \mathcal{L}(\varepsilon, su_{\varepsilon} + (1 - s)u_{0}, q_{\varepsilon})(\varphi) \, ds = 0 \quad \text{for all } \varphi \in \mathcal{V}.$$
(2.21)

In addition, plugging $\varphi = u_{\varepsilon} - u_0$ into (2.22), one obtains $\mathcal{L}(\varepsilon, u_{\varepsilon}, 0) = \mathcal{L}(\varepsilon, u_0, q_{\varepsilon})$ for $\varepsilon > 0$, so the Lagrangian only depends on the unperturbed state u_0 and the averaged adjoint variable q_{ε} . We henceforth assume that the averaged adjoint equation admits a unique solution and denote as q_0 the unperturbed averaged adjoint state satisfying

$$\int_0^1 \partial_u \mathcal{L}(0, su_0 + (1 - s)u_0, q_0)(\varphi) \, ds = 0 \quad \text{for all } \varphi \in \mathcal{V}.$$
(2.22)

Proposition 2.4.

(1) Let $\ell_1 : \mathbf{R}^+ \to \mathbf{R}^+$ be a function with $\lim_{\epsilon \searrow 0} \ell_1(\epsilon) = 0$. Furthermore, assume that the limits

$$\mathcal{R}^{(1)}(u_0, q_0) := \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_0, q_\varepsilon) - \mathcal{L}(\varepsilon, u_0, q_0)}{\ell_1(\varepsilon)},$$
(2.23)

 $\partial_{\ell}^{(1)}\mathcal{L}(0,u_0,q_0) := \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon,u_0,q_0) - \mathcal{L}(0,u_0,q_0)}{\ell_1(\varepsilon)},$ (2.24)

exist. Then we have the following expansion

$$j(\varepsilon) = j(0) + \ell_1(\varepsilon) \Big(\mathcal{R}^{(1)}(u_0, q_0) + \partial_{\ell}^{(1)} \mathcal{L}(0, u_0, q_0) \Big) + o(\ell_1(\varepsilon)).$$
(2.25)

(2) Let $\ell_2 : \mathbf{R}^+ \to \mathbf{R}^+$ be a function with $\lim_{\varepsilon \searrow 0} \frac{\ell_2(\varepsilon)}{\ell_1(\varepsilon)} = 0$. Furthermore, assume that the assumption under (1) holds and the limits

$$\mathcal{R}^{(2)}(u_0, q_0) := \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_0, q_\varepsilon) - \mathcal{L}(\varepsilon, u_0, q_0) - \ell_1(\varepsilon) \mathcal{R}^{(1)}(u_0, q_0)}{\ell_2(\varepsilon)},$$
(2.26)

$$\partial_{\ell}^{(2)} \mathcal{L}(0, u_0, q_0) := \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_0, q_0) - \mathcal{L}(0, u_0, q_0) - \ell_1(\varepsilon) \partial_{\ell}^{(1)} \mathcal{L}(0, u_0, q_0)}{\ell_2(\varepsilon)}, \quad (2.27)$$

exist. Then we have the following expansion

$$egin{aligned} \dot{j}(arepsilon) &= \dot{j}(0) + \ell_1(arepsilon) \Big(\mathcal{R}^{(1)}(u_0,q_0) + \partial_\ell^{(1)} \mathcal{L}(0,u_0,q_0) \Big) + \ell_2(arepsilon) \Big(\mathcal{R}^{(2)}(u_0,q_0) \\ &+ \partial_\ell^{(2)} \mathcal{L}(0,u_0,q_0) \Big) + o(\ell_2(arepsilon)). \end{aligned}$$

Proof. ad (1): Recalling $\mathcal{L}(\varepsilon, u_{\varepsilon}, 0) = \mathcal{L}(\varepsilon, u_0, q_{\varepsilon})$ we have

$$\begin{split} j(\varepsilon) - j(0) &= \mathcal{L}(\varepsilon, u_{\varepsilon}, 0) - \mathcal{L}(0, u_0, 0) \\ &= \mathcal{L}(\varepsilon, u_0, q_{\varepsilon}) - \mathcal{L}(0, u_0, q_0) \\ &= \mathcal{L}(\varepsilon, u_0, q_{\varepsilon}) - \mathcal{L}(\varepsilon, u_0, q_0) + \mathcal{L}(\varepsilon, u_0, q_0) - \mathcal{L}(0, u_0, q_0). \end{split}$$

Dividing by $\ell^1(\varepsilon)$ for $\varepsilon > 0$ and passing to the limit $\varepsilon \searrow 0$ yields the result. ad (2): Similar to item (1).

The previous result can be readily generalised to compute the nth-order topological derivative as shown in the following proposition.

Proposition 2.5. (nth topological derivative). Assume that the following hypotheses hold.

(1) There exist numbers $\delta a^{(i)}$ and $\delta f^{(i)}$, i = 1, 2, ..., n and a function $\ell_1 : \mathbf{R}^+ \to \mathbf{R}^+$ with $\lim_{\epsilon \searrow 0} \ell_1(\epsilon) = 0$, such that n-1

$$(a_{\varepsilon} - a_0)(u_0, q_0) = \ell_1(\varepsilon) \sum_{i=0}^{n-1} \varepsilon^i \delta a^{(i+1)} + o(\varepsilon^n \ell_1(\varepsilon)), \qquad (2.28)$$

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$$(f_{\varepsilon} - f_0)(u_0) = \ell_1(\varepsilon) \sum_{i=0}^{n-1} \varepsilon^i \delta f^{(i+1)} + o(\varepsilon^n \ell_1(\varepsilon)), \qquad (2.29)$$

$$(J_{\varepsilon} - J_0)(u_0) = \ell_1(\varepsilon) \sum_{i=0}^{n-1} \varepsilon^i \delta J^{(i+1)} + o(\varepsilon^n \ell_1(\varepsilon)),$$
(2.30)

(2) There exist numbers $\delta A^{(i)}$ and $\delta F^{(i)}$, i = 1, 2, ..., n, such that

$$(a_{\varepsilon} - a_0)(u_0, q_{\varepsilon} - q_0) = \ell_1(\varepsilon) \sum_{i=0}^{n-1} \varepsilon^i \delta A^{(i+1)} + o(\varepsilon^n \ell_1(\varepsilon)),$$
(2.31)

$$(f_{\varepsilon} - f_0)(q_{\varepsilon} - q_0) = \ell_1(\varepsilon) \sum_{i=0}^{n-1} \varepsilon^i \delta F^{(i+1)} + o(\varepsilon^n \ell_1(\varepsilon)),$$
(2.32)

where $q_{\varepsilon} \in \mathcal{V}$ is the averaged adjoint state satisfying

$$a_{\varepsilon}(\varphi, v_{\varepsilon}) = -\int_{0}^{1} \partial J_{\varepsilon}(su_{\varepsilon} + (1 - s)u_{0})(\varphi) \, ds \quad \text{for all } \varphi \in \mathcal{W}.$$
(2.33)

Then the following expansion holds

$$J_{\varepsilon}(u_{\varepsilon}) = J_{0}(u_{0}) + \ell_{1}(\varepsilon) \sum_{i=0}^{n-1} \varepsilon^{i} \left(\delta a^{(i+1)} - \delta f^{(i+1)} + \delta A^{(i+1)} - \delta F^{(i+1)} \right) + o(\varepsilon^{n} \ell_{1}(\varepsilon)).$$
(2.34)

Proof. Similar to the proof of Proposition 2.4, we write

$$J_{\varepsilon}(u_{\varepsilon}) - J_0(u_0) = \mathcal{L}(\varepsilon, u_0, q_{\varepsilon}) - \mathcal{L}(\varepsilon, u_0, q_0) + \mathcal{L}(\varepsilon, u_0, q_0) - \mathcal{L}(0, u_0, q_0).$$
(2.35)

The second term on the right-hand side reads

$$\mathcal{L}(\varepsilon, u_0, q_0) - \mathcal{L}(0, u_0, q_0) = (J_{\varepsilon} - J_0)(u_0) + (a_{\varepsilon} - a_0)(u_0, q_0) - (f_{\varepsilon} - f_0)(u_0).$$
(2.36)

So using (2.28)–(2.30), we can expand each difference in this expression. As for the first difference on right-hand side, one has

$$\mathcal{L}(\varepsilon, u_0, q_{\varepsilon}) - \mathcal{L}(\varepsilon, u_0, q_0) = \underbrace{(a_{\varepsilon} - a_0)(u_0, q_{\varepsilon} - q_0) - (f_{\varepsilon} - f_0)(q_{\varepsilon} - q_0)}_{=0} + \underbrace{a_0(u_0, q_{\varepsilon} - q_0) - f_0(q_{\varepsilon} - q_0)}_{=0}.$$

Therefore, employing (2.31), (2.32), we can also expand these two differences and obtain the claimed formula (2.34).

Remark 2.6.

(1) Checking the expansions (2.24), (2.27) in applications usually requires some regularity of the state u_0 and adjoint state $q_0 = p_0$. However, the computation of this expansion is a straightforward application of Taylor's formula. The reader will find an application in Section 5.2

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EC 39,1 (2) The computation of the asymptotic expansions (2.23), (2.26) requires the study of the asymptotic behaviour of q_e and therefore also of u_e . This is the most difficult part and can be done by the compounded layer expansion involving corrector equations (see for instance, Mazya *et al.*, 2000b; Mazya *et al.*, 2000a) as is presented in Section 4.2

2.4 Delfour's method

In this section we discuss a method proposed by M.C. Delfour in (Delfour, 2018, Thm.3.3). The definite advantage is that it uses the unperturbed adjoint equation and only requires the asymptotic analysis of the state equation, but it seems to come with the shortcoming that it is only applicable to certain cost functions; see Gangl and Sturm (2020a). As before, we let \mathcal{L} be a Lagrangian function and denote as u_{ε} the perturbed state equation (solution to (2.1) for $\varepsilon \geq 0$) and p_0 the unperturbed adjoint equation (solution to (2.6) for $\varepsilon = 0$). Using the perturbed state and the unperturbed adjoint equation, Delfour proposed the following result for computing the first-order topological derivative, where we also incorparate the second-order topological derivative.

Proposition 2.7. (Delfour, 2018).

(1) Let $\ell_1 : \mathbf{R}^+ \to \mathbf{R}^+$ be a function with $\ell_1 \ge 0$ and $\lim_{\epsilon \searrow 0} \ell_1(\epsilon) = 0$. Furthermore, assume that the limits

$$\mathcal{R}_{1}^{(1)}(u_{0},p_{0}) := \lim_{\varepsilon \searrow 0} \frac{1}{\ell_{1}(\varepsilon)} [\mathcal{L}(\varepsilon,u_{\varepsilon},p_{0}) - \mathcal{L}(\varepsilon,u_{0},p_{0}) - \mathcal{L}(\varepsilon,u_{0},p_{0})(u_{\varepsilon}-u_{0})], \quad (2.37)$$

$$\mathcal{R}_{2}^{(1)}(u_{0},p_{0}) := \lim_{\varepsilon \searrow 0} \frac{1}{\ell_{1}(\varepsilon)} (\partial_{u} \mathcal{L}(\varepsilon,u_{0},p_{0}) - \partial_{u} \mathcal{L}(0,u_{0},p_{0}))(u_{\varepsilon} - u_{0}), \qquad (2.38)$$

$$\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0) := \lim_{\epsilon \to 0} \frac{1}{\ell_1(\epsilon)} (\mathcal{L}(\epsilon, u_0, p_0) - \mathcal{L}(0, u_0, p_0)),$$
(2.39)

exist. Then the following expansion holds:

$$j(\varepsilon) = j(0) + \ell_1(\varepsilon) \Big(\mathcal{R}_1^{(1)}(u_0, p_0) + \mathcal{R}_2^{(1)}(u_0, p_0) + \partial_\ell^{(1)} \mathcal{L}(0, u_0, p_0) \Big) + o(\ell_1(\varepsilon)).$$
(2.40)

(2) Let $\ell_2 : \mathbf{R}^+ \to \mathbf{R}^+$ be a function with $\ell_2 \ge 0$ and $\lim_{\epsilon \to 0} \frac{\ell_2(\epsilon)}{\ell_1(\epsilon)} = 0$. Furthermore, assume that the assumptions under (1) hold and that the limits

$$\mathcal{R}_{1}^{(2)}(u_{0},p_{0}) \coloneqq \lim_{\varepsilon \searrow 0} \frac{1}{\ell_{2}(\varepsilon)} \left[\mathcal{L}(\varepsilon,u_{\varepsilon},p_{0}) - \mathcal{L}(\varepsilon,u_{0},p_{0}) - \mathcal{L}(\varepsilon,u_{0},p_{0})(u_{\varepsilon}-u_{0}) - \ell_{1}(\varepsilon)\mathcal{R}_{1}^{(1)}(u_{0},p_{0}) \right],$$

$$(2.41)$$

$$\mathcal{R}_{2}^{(2)}(u_{0},p_{0}) \coloneqq \lim_{\varepsilon \searrow 0} \frac{1}{\ell_{2}(\varepsilon)} \left[(\partial_{u}\mathcal{L}(\varepsilon,u_{0},p_{0}) - \partial_{u}\mathcal{L}(0,u_{0},p_{0}))(u_{\varepsilon} - u_{0}) - \ell_{1}(\varepsilon)\mathcal{R}_{2}^{(1)}(u_{0},p_{0}) \right],$$

$$(2.42)$$

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$$\underbrace{\mathsf{EC}}_{39,1} \qquad \qquad \partial_{\ell}^{(2)} \mathcal{L}(0, u_0, p_0) := \lim_{\varepsilon \searrow 0} \frac{1}{\ell_2(\varepsilon)} \Big[\mathcal{L}(\varepsilon, u_0, p_0) - \mathcal{L}(0, u_0, p_0) - \ell_1(\varepsilon) \partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0) \Big], \quad (2.43)$$

exist. Then, we have the following expansion:

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$$j(\varepsilon) = j(0) + \ell_1(\varepsilon) \Big(\mathcal{R}_1^{(1)}(u_0, p_0) + \mathcal{R}_2^{(1)}(u_0, p_0) + \partial_\ell^{(1)} \mathcal{L}(0, u_0, p_0) \Big) + \ell_2(\varepsilon) \Big(\mathcal{R}_1^{(2)}(u_0, p_0) + \mathcal{R}_2^{(2)}(u_0, p_0) + \partial_\ell^{(2)} \mathcal{L}(0, u_0, p_0) \Big) + o(\ell_2(\varepsilon)).$$
(2.44)

Proof. ad (1): Firstly, note that by definition the unperturbed adjoint state p_0 satisfies

$$\partial_u \mathcal{L}(0, u_0, p_0)(\varphi) = 0 \quad \text{for } \varphi \in \mathcal{W}$$

Thus, we can write $j(\varepsilon) - j(0)$ in the following way:

$$j(\varepsilon) - j(0) = \mathcal{L}(\varepsilon, u_{\varepsilon}, 0) - \mathcal{L}(0, u_0, 0)$$

$$= \mathcal{L}(\varepsilon, u_{\varepsilon}, p_0) - \mathcal{L}(0, u_0, p_0)$$

$$= \mathcal{L}(\varepsilon, u_{\varepsilon}, p_0) - \mathcal{L}(\varepsilon, u_0, p_0) - \partial_u \mathcal{L}(\varepsilon, u_0, p_0)(u_{\varepsilon} - u_0)$$

$$+ \partial_u \mathcal{L}(\varepsilon, u_0, p_0)(u_{\varepsilon} - u_0) - \partial_u \mathcal{L}(0, u_0, p_0)(u_{\varepsilon} - u_0)$$

$$+ \mathcal{L}(\varepsilon, u_0, p_0) - \mathcal{L}(0, u_0, p_0).$$
(2.45)

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Now, dividing by $\ell_1(\varepsilon)$, $\varepsilon > 0$ and passing to the limit $\varepsilon \searrow 0$ yield the result. ad (2): This can be shown similarly to (1).

Remark 2.8. Similarly to Amstutz' method and the averaged adjoint method, Delfour's method requires the asymptotic behaviour of u_{ε} on the whole domain to compute (2.37), (2.41). This may be challenging in the analysis in dimension two for some cost functionals. Additionally, (2.38), (2.42) can be checked by smoothness assumptions on p_0 and u_0 and the knowledge of the asymptotics of u_{ε} on a small subset of size ε . The remaining terms (2.39), (2.43) usually are computed making use of Taylor's expansion of u_0 and p_0 , respectively.

2.4.1 Overview of the employed adjoint equations. The methods reviewed in the previous sections make use of three different adjoint equations. The method of Amstutz (2006a) uses an adjoint equation which depends on the unperturbed state variable:

$$p_{\varepsilon} \in \mathcal{W}: \ \partial_{u}\mathcal{L}(\varepsilon, u_{0}, p_{\varepsilon})(\varphi) = 0 \quad \text{for all } \varphi \in \mathcal{V}.$$

Delfour's method uses the unperturbed adjoint equation:

$$p_0 \in \mathcal{W}: \ \partial_u \mathcal{L}(0, u_0, p_0)(\varphi) = 0 \quad \text{for all } \varphi \in \mathcal{V}.$$

Finally, there is the averaged adjoint method, which employs the averaged adjoint equation Sturm (2015) and Delfour and Sturm (2016):

$$q_{\varepsilon} \in \mathcal{W}: \int_{0}^{1} \partial_{u} \mathcal{L}(\varepsilon, su_{\varepsilon} + (1 - s)u_{0}, q_{\varepsilon})(\varphi) \, ds = 0 \quad \text{for all } \varphi \in \mathcal{V}.$$

3. Analysis of the perturbed state equation

Let $\Omega \subset D$ open, $\omega \subset \mathbb{R}^d$ be a bounded domain containing the origin $0 \in \omega$ and let $x_0 \in D$. Moreover, we define the perturbation $\omega_{\varepsilon} := x_0 + \varepsilon \omega$ for $\varepsilon \ge 0$ at x_0 . Consider the perturbed state solution of (1.2) for $\Omega = \omega_{\varepsilon}$, that is, find $u_{\varepsilon} \in H^1(D)^d$, such that $u_{\varepsilon}|_{\Gamma} = u_D$ and

$$\int_{\mathsf{D}} \mathbf{C}_{\omega_{\epsilon}} \boldsymbol{\epsilon}(u_{\epsilon}) : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \ dx = \int_{\mathsf{D}} f_{\omega_{\epsilon}} \cdot \boldsymbol{\varphi} \ dx + \int_{\Gamma_{N}} u_{N} \cdot \boldsymbol{\varphi} \ dS \quad \text{for all } \boldsymbol{\varphi} \in H^{1}_{\Gamma}(\mathsf{D})^{d}.$$
(3.1)

In the following sections we are going to derive the asymptotic expansion of u_{ε} using the compounded layer method; see, Mazya *et al.* (2000a, b). We note that this expansion has already been computed in Bonnet and Cornaggia (2017) by means of Green's function and earlier in Ammari *et al.* (2002) for $f_{\Omega} = 0$. In the following two sections we state some preliminary results regarding the scaling of inequalities and remainder estimates, which will be needed later on.

3.1 Scaling of inequalities

In this section we discuss the influence of a parametrised affine transformation $\Phi_{\varepsilon}: \mathbf{R}^d \to \mathbf{R}^d$ onto norms and the scaling behaviour of some well-known inequalities with respect to that parameter.

Definition 3.1. For $\varepsilon > 0$ we define the inflation of D by $D_{\varepsilon} := \Phi_{\varepsilon}^{-1}(D)$, where the affine linear transformation Φ_{ε} is given by $\Phi_{\varepsilon}(x) := x_0 + \varepsilon x$, for a fixed point $x_0 \in D$.

For convenience, we denote the inflated boundary $\Gamma_{\varepsilon} := \Phi_{\varepsilon}^{-1}(\Gamma)$ as well as $\Gamma_{N,\varepsilon} := \Phi_{\varepsilon}^{-1}(\Gamma_N)$ and $\Gamma_{m,\varepsilon} := \Phi_{\varepsilon}^{-1}(\Gamma_m)$. Since Φ_{ε} is a bi-Lipschitz continuous map, it holds $\varphi \in H_{\Gamma}^1(\mathsf{D})^d$ if and only if $\varphi \bigcirc \Phi_{\varepsilon} \in H_{\Gamma_{\varepsilon}}^1(\mathsf{D}_{\varepsilon})^d$; see (Ziemer, 1989, p. 52, Thm.2.2.2). Furthermore, since the transformation Φ_{ε} leads to a sclaing of the H^1 norm, we use the following notation.

Definition 3.2. For $\varepsilon > 0$ and $\varphi \in H^1(\mathsf{D}_{\varepsilon})^d$ let

$$\|\varphi\|_{\varepsilon} := \varepsilon \|\varphi\|_{L_2(\mathsf{D}_{\varepsilon})^d} + \| \nabla \varphi\|_{L_2(\mathsf{D}_{\varepsilon})^{d \times d}}.$$
(3.2)

Lemma 3.3. Let $D \subset \mathbf{R}^d$ be a bounded Lipschitz domain and let $\varepsilon > 0$.

(1) For $1 \le p < \infty$ and $\varphi \in L_p(\mathsf{D}_{\varepsilon})^d$ there holds

$$\varepsilon^{\frac{p}{b}} \|\varphi\|_{L_{p}(\mathsf{D}_{\varepsilon})^{d}} = \|\varphi \circ \Phi_{\varepsilon}^{-1}\|_{L_{p}(\mathsf{D})^{d}}.$$
(3.3)

(2) For $1 \le p < \infty$ and $\varphi \in W_{p}^{1}(\mathsf{D}_{\varepsilon})^{d}$ there holds

$$\varepsilon_{p}^{d-1} \| \cdot \nabla \varphi \|_{L_{p}(\mathsf{D}_{\varepsilon})^{d \times d}} = \| \cdot \nabla \left(\varphi \circ \Phi_{\varepsilon}^{-1} \right) \|_{L_{p}(\mathsf{D})^{d \times d}}.$$
(3.4)

(3) For $\varphi \in H^1(\mathsf{D}_{\varepsilon})^d$ there holds

$$\|\boldsymbol{\varphi} \circ \boldsymbol{\Phi}_{\varepsilon}^{-1}\|_{H^{1}(\mathsf{D})^{d}} = \varepsilon^{\frac{d}{2}-1} \|\boldsymbol{\varphi}\|_{\varepsilon}.$$
(3.5)

Proof.

(1) A change of variables yields

$$\|\varphi\|_{L_{p}(\mathsf{D}_{\varepsilon})^{d}}^{p} = \varepsilon^{-d} \int_{\mathsf{D}} |\varphi \circ \Phi_{\varepsilon}^{-1}|^{p} dx = \varepsilon^{-d} \|\varphi \circ \Phi_{\varepsilon}^{-1}\|_{L_{p}(\mathsf{D})^{d}}^{p},$$
(3.6)

where we used $|\det(\nabla \Phi_{\varepsilon}^{-1})| = \varepsilon^{-d}$.

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EC (2) Taking into account that $\nabla(\varphi \circ \Phi_{\varepsilon}^{-1}) = \varepsilon^{-1} \nabla \varphi \circ \Phi_{\varepsilon}^{-1}$, a change of variables yields (39,1) $\|\nabla \varphi\|_{L_{p}(\mathbb{D}_{\varepsilon})^{d \times d}}^{p} = \varepsilon^{-d} \int_{\mathbb{D}} |\nabla \varphi \circ \Phi_{\varepsilon}^{-1}|^{p} dx = \varepsilon^{-d} \varepsilon^{p} \int_{\mathbb{D}} |\nabla (\varphi \circ \Phi_{\varepsilon}^{-1})|^{p} dx = \varepsilon^{p-d} \|\nabla (\varphi \circ \Phi_{\varepsilon}^{-1})\|_{L_{p}(\mathbb{D})^{d \times d}}^{p}.$ (3.7)

(3) This follows from item (1) and (2).

Lemma 3.4. Let $D \subset \mathbf{R}^d$ be a bounded Lipschitz domain, $\Gamma \subset \partial D$ and let $\varepsilon > 0$. Recall the definitions $D_{\varepsilon} = \Phi_{\varepsilon}^{-1}(D)$ and $\Gamma_{\varepsilon} = \Phi_{\varepsilon}^{-1}(\Gamma)$.

- (1) For $1 \le p \le q \le \infty$, there exists a constant C > 0, such that $\|\varphi\|_{L_p(D_e)^d} \le C \varepsilon^{\frac{d}{q} - \frac{d}{p}} \|\varphi\|_{L_q(D_e)^d}.$ (3.8)
- (2) Let $d \ge 3$ and 2^* denote the Sobolev conjugate of 2. There exists a constant C > 0, such that

$$\|\varphi\|_{L_2^*(\mathsf{D}_\varepsilon)^d} \le C \|\varphi\|_{\varepsilon}. \tag{3.9}$$

- (3) Let d = 2 and $\alpha > 0$ small. There exists a constant C > 0 and $\delta > 0$ small, such that $\|\varphi\|_{L_{(2-\delta)}^*(D_{\varepsilon})^d} \le C\varepsilon^{-\alpha} \|\varphi\|_{\varepsilon}.$ (3.10)
- (4) For $\varphi \in H^1(\mathsf{D}_{\varepsilon})^d$ we have

$$\|\varphi\|_{L_2(\Gamma_\varepsilon)^d} \le C\varepsilon^{-\frac{1}{2}} \|\varphi\|_\varepsilon. \tag{3.11}$$

(5) Given a smooth connected domain Γ ⊂ ∂D, there is a continuous extension operator Z_{Γ_ε} : H¹/₂(Γ_ε)^d → H¹(D_ε)^d, such that

$$\|Z_{\Gamma_{\varepsilon}}(\varphi)\|_{\varepsilon} \leq C(\varepsilon^{\frac{1}{2}} \|\varphi\|_{L_{2}(\Gamma_{\varepsilon})^{d}} + |\varphi|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}}), \quad \text{for all } \varphi \in H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}, \tag{3.12}$$

where C > 0 is independent of ε .

(6) Let $\Gamma \subset \partial D$ have positive measure. There exists a constant C > 0, such that

$$\|\varphi\|_{L_2(\mathsf{D}_{\varepsilon})^d} \le C\varepsilon^{-1} \|\nabla\varphi\|_{L_2(\mathsf{D}_{\varepsilon})^{d\times d}}, \quad \text{for all } \varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d.$$
(3.13)

Proof.

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- (1) This is a direct consequence of Lemma 3.3 item (1).
- (2) We use Lemma 3.3 item (1) and (2) and apply the Gagliardo–Nirenberg inequality (Evans, 2010, p. 265, Thm. 2) to the bounded domain D.

$$\begin{aligned} \|\varphi\|_{L_{\frac{2}{2}}(\mathbb{D}_{\varepsilon})^{d}} &= \varepsilon^{-\frac{d}{2}} \|\varphi \circ \Phi_{\varepsilon}^{-1}\|_{L_{\frac{2}{2}}(\mathbb{D})^{d}} & \text{Adjoint-based} \\ &\leq C\varepsilon^{-\frac{d}{2}} \|\varphi \circ \Phi_{\varepsilon}^{-1}\|_{H^{1}(\mathbb{D})^{d}} & (3.14) \\ &= C\varepsilon^{\frac{d}{2}-\frac{d}{2}-1} \|\varphi\|_{\varepsilon}. & \textbf{73} \end{aligned}$$

Now the result follows from $\frac{d}{2} - \frac{d}{2^*} = 1$.

(3) We apply the Gagliardo–Nirenberg inequality with respect to $p := 2 - \delta < 2$ and use the continuous embedding $L_2(D) \hookrightarrow L_{2-\delta}(D)$ on the bounded domain D:

$$\begin{aligned} \|\varphi\|_{L_{(2-\delta)}^{*}(\mathsf{D}_{\varepsilon})^{d}} &= \varepsilon^{-\frac{2}{(2-\delta)^{*}}} \|\varphi \circ \Phi_{\varepsilon}^{-1}\|_{L_{(2-\delta)}^{*}(\mathsf{D})^{d}} \\ &\leq C \varepsilon^{-\frac{2}{(2-\delta)^{*}}} \left(\left\|\varphi \circ \Phi_{\varepsilon}^{-1}\right\|_{L_{(2-\delta)}(\mathsf{D})^{d}} + \left\|\nabla\left(\varphi \circ \Phi_{\varepsilon}^{-1}\right)\right\|_{L_{(2-\delta)}(\mathsf{D})^{d\times d}} \right) \\ &\leq C \varepsilon^{-\frac{2}{(2-\delta)^{*}}} \left(\left\|\varphi \circ \Phi_{\varepsilon}^{-1}\right\|_{L_{2}(\mathsf{D})^{d}} + \left\|\nabla\left(\varphi \circ \Phi_{\varepsilon}^{-1}\right)\right\|_{L_{2}(\mathsf{D})^{d\times d}} \right) \\ &= C \varepsilon^{-\frac{2}{(2-\delta)^{*}}} \|\varphi\|_{\varepsilon}. \end{aligned}$$
(3.15)

Since $(2 - \delta)^*$ diverges to ∞ as $\delta \searrow 0$, the result follows.

- (4) This follows from a change of variables and the continuity of the trace operator.
- (5) From (Wloka, 1987, p. 129, Thm. 8.8), we know there exists a continuous extension operator $Z_{\Gamma}: H^{\frac{1}{2}}(\Gamma)^d \to H^1(\mathsf{D})^d$. Thus, a scaling argument similar to the previous ones yields the result.
- Items (1) and (2) of Lemma 3.3 and an application of Friedrich's inequality yield the (6) result.

3.2 Remainder estimates

We begin this section with the following auxiliary result.

Lemma 3.5. Let $V : \mathbf{R}^d \to \mathbf{R}^d \in H^1_{loc}(\mathbf{R}^d)^d$ satisfy

$$|V(x)| = c_1 |x|^{-m} + \mathcal{O}\Big(|x|^{-m-1}\Big), \quad |\nabla V(x)| = c_2 |x|^{-m-1} + \mathcal{O}\Big(|x|^{-m-2}\Big), \tag{3.16}$$

for $x \in B_{\delta}(0)^{c}$, where $\delta > 0$ is fixed, $m \in \mathbf{R}$ and $c_1, c_2 > 0$ are constants. Then there is a constant C > 0, such that for $\Gamma \subset \partial D$ and $\varepsilon > 0$ sufficiently small the following estimates hold:

- (1) $\|V\|_{L_2(\Gamma_c)^d} \leq C \varepsilon^{\frac{2m+1-d}{2}}$.
- (2) $|V|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}} \leq C\varepsilon^{\frac{2m+2-d}{2}}.$ (3) $\|\nabla V\|_{L_{2}(\Gamma_{\varepsilon})^{d \times d}} \leq C\varepsilon^{\frac{2m+3-d}{2}}.$

Proof.

(1) Let $M := \min_{x \in \Gamma} |x - x_0| > 0$ and ε sufficiently small, such that the leading term of *V* dominates the remainder for $x \in \Gamma^{\varepsilon}$. Then we conclude

$$\|V\|_{L_2(\Gamma_{\varepsilon})^d}^2 = \int_{\Gamma_{\varepsilon}} |V|^2 \, dS \le |\Gamma_{\varepsilon}| \left(\varepsilon^{-1}M\right)^{-2m} \le C\varepsilon^{1-d+2m}. \tag{3.17}$$

Now taking the square root shows the result.

(2) Let $0 < r_1 < r_2$ such that $\partial D \subset S$, where $S := B_{r_2}(x_0) \setminus B_{r_1}(x_0)$. Additionally, let ε be sufficiently small, such that $\rho < \varepsilon^{-1}r_1$. Now we apply a change of variables to integrate over the fixed domain and split the norm into two terms, which are treated separately. Therefore, fix some $\delta > 0$ sufficiently small. Then

$$\begin{split} \left|V\right|_{H^{\frac{1}{2}}(\partial D_{\varepsilon})^{d}}^{2} &= \int_{\partial D_{\varepsilon}} \int_{\partial D_{\varepsilon}} \frac{\left|V(x) - V(y)\right|^{2}}{\left|x - y\right|^{d}} \, dS_{y} dS_{x} \\ &= \varepsilon^{2-2d} \int_{\partial D} \int_{\partial D} \int_{\partial D} \frac{\left|V\left(\Phi_{\varepsilon}^{-1}(x)\right) - V\left(\Phi_{\varepsilon}^{-1}(y)\right)\right|^{2}}{\left|\Phi_{\varepsilon}^{-1}(x) - \Phi_{\varepsilon}^{-1}(y)\right|^{d}} \, dS_{y} dS_{x} \\ &= \varepsilon^{2-d} \int_{\partial D} \int_{\partial D} \frac{\left|V\left(\Phi_{\varepsilon}^{-1}(x)\right) - V\left(\Phi_{\varepsilon}^{-1}(y)\right)\right|^{2}}{\left|x - y\right|^{d}} \, dS_{y} dS_{x} \\ &= \varepsilon^{2-d} \int_{\partial D} \int_{\partial D \setminus B_{\delta}(x)} \frac{\left|V\left(\Phi_{\varepsilon}^{-1}(x)\right) - V\left(\Phi_{\varepsilon}^{-1}(y)\right)\right|^{2}}{\left|x - y\right|^{d}} \, dS_{y} dS_{x} \end{split}$$
(3.18)

$$+ \varepsilon^{2-d} \int_{\partial D} \int_{\partial D \cap B_{\delta}(x)} \frac{|V(\Phi_{\varepsilon}^{-1}(x)) - V(\Phi_{\varepsilon}^{-1}(y))|^{2}}{|x - y|^{d}} \, dS_{y} dS_{x}.$$
(3.19)

In order to compute the first term (3.18), we consider for each pair $(x, y) \in \partial D \times \partial D$ a smooth path $\varphi_{x,y}:[0, 1] \to S$ satisfying $\varphi_{x,y}(0) = x$ and $\varphi_{x,y}(1) = y$. Since *V* is smooth in $\Phi_{\varepsilon}^{-1}(S)$, we can apply the mean value theorem to the function $F(t) := V(\Phi_{\varepsilon}^{-1}(\varphi_{x,y}(t)))$ and consider $\nabla(\Phi_{\varepsilon}^{-1}) = \varepsilon^{-1}I_d$ to get

$$V\left(\Phi_{\varepsilon}^{-1}(y)\right) - V\left(\Phi_{\varepsilon}^{-1}(x)\right) = \int_{0}^{1} \varepsilon^{-1} \nabla V\left(\Phi_{\varepsilon}^{-1}\left(\varphi_{x,y}(s)\right)\right) \varphi_{x,y}'(s) \ ds.$$
(3.20)

Thus, by Hölder's inequality we conclude

$$|V(\Phi_{\varepsilon}^{-1}(y)) - V(\Phi_{\varepsilon}^{-1}(x))| \le \varepsilon^{-1} \|\nabla V(\Phi_{\varepsilon}^{-1}(\varphi_{xy}(\cdot)))\|_{L^{\infty}(0,1)^{d \times d}} \|\varphi_{xy}'\|_{L^{1}(0,1)^{d}}.$$
 (3.21)

Since this inequality holds for every smooth path $\varphi_{x,y}$ connecting *x* and *y*, the estimate holds for $d_S(x, y) := \inf_{\varphi_{x,y}[0,1] \to S} \|\varphi'_{x,y}\|_{L^1(0,1)^d}$. Furthermore, since *S* is bounded and path connected, the following estimate holds (see Delfour and Zolésio, 2011, Thm 5.8).

$$d_S(x,y) \le C|x-y|, \quad \text{for } x, y \in S \tag{3.22}$$

for some constant C > 0 that only depends on *S*. Additionally, considering the representation formula of *V*, we have $\|\nabla V(x)\| = c_2 |x|^{-m-1} + O(|x|^{-m-2})$. Hence, choosing ε small enough,

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EC 39.1 such that the leading order term dominates the remainder, we get

$$\|\nabla U^{(1)}\left(\Phi_{\varepsilon}^{-1}\left(\varphi_{x,y}(s)\right)\right)\|_{L^{\infty}(0,1)^{d\times d}} \leq \max_{z\in\overline{S}} |\nabla U^{(1)}\left(\Phi_{\varepsilon}^{-1}(z)\right)| \leq C\varepsilon^{m+1}.$$
(3.23) methods

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As a result, we conclude

$$\varepsilon^{2-d} \int_{\partial D} \int_{\partial D \setminus B_{\delta}(x)} \frac{|V(\Phi_{\varepsilon}^{-1}(y)) - V(\Phi_{\varepsilon}^{-1}(x))|^{2}}{|x - y|^{d}} dS_{y} dS_{x}$$

$$\leq \varepsilon^{-d} \int_{\partial D} \int_{\partial D \setminus B_{\delta}(x)} \frac{C\varepsilon^{2m+2}|x - y|^{2}}{|x - y|^{d}} dS_{y} dS_{x}$$

$$\leq \varepsilon^{-d} \int_{\partial D} \int_{\partial D \setminus B_{\delta}(x)} \frac{C\varepsilon^{2m+2}}{\delta^{d-2}} dS_{y} dS_{x}$$

$$\leq C\varepsilon^{2m+2-d}.$$
(3.24)

The key here was to choose the set *S* such that $\Phi_{\varepsilon}^{-1} \bigcirc \varphi_{x,y}([0,1]) \subset B_{\rho}(0)^{c}$ for every path $\varphi_{x,y}$. The second term (3.19) can be estimated by using a straight line connecting $x \in \partial D$ and $y \in \partial D$. Therefore, let $\varphi_{x,y}(t) := x + t(y - x)$, for $t \in [0, 1]$. Since we only need to consider $(x, y) \in \partial D \times \partial D$ such that $|x - y| < \delta$, $\Phi_{\varepsilon}^{-1} \bigcirc \varphi_{x,y}([0,1]) \subset B_{\rho}(0)^{c}$ can be guaranteed by choosing δ sufficiently small. Again, an application of the mean value theorem yields

$$|V(\Phi_{\varepsilon}^{-1}(x)) - V(\Phi_{\varepsilon}^{-1}(y))|^{2} \le \varepsilon^{-2} \max_{z \in \overline{S_{\delta}}} |\nabla V(\Phi_{\varepsilon}^{-1}(z))|^{2} |x - y|^{2},$$
(3.25)

where $S_{\delta} := \bigcup_{x \in \partial D} B_{\delta}(x)$. Furthermore, a similar estimation to (3.23) yields

$$\max_{z \in \overline{S_{\delta}}} |\nabla V \left(\Phi_{\varepsilon}^{-1}(z) \right)|^2 \le C \varepsilon^{2m+2}.$$
(3.26)

Plugging this estimate into (3.19), yields

$$\varepsilon^{2-d} \int_{\partial D} \int_{\partial D \cap B_{\delta}(x)} \frac{|V(\Phi_{\varepsilon}^{-1}(x)) - V(\Phi_{\varepsilon}^{-1}(y))|^{2}}{|x - y|^{d}} dS_{y} dS_{x}$$

$$\leq \varepsilon^{-d} \int_{\partial D} \int_{\partial D \cap B_{\delta}(x)} \frac{\max_{z \in \overline{S}_{\delta}} |\nabla V(\Phi_{\varepsilon}^{-1}(z))|^{2}}{|x - y|^{d-2}} dS_{y} dS_{x}$$

$$\leq C \varepsilon^{2m+2-d} \int_{\partial D} \int_{\partial D \cap B_{\delta}(x)} \frac{1}{|x - y|^{d-2}} dy dx.$$
(3.27)

To finish our proof, we need to show that the integral on the right-hand side is finite. Therefore, let $\hat{A}_j(x) := B_{2^{(1-j)}\delta}(x) \setminus B_{2^{-j}\delta}(x)$, for $j \in \mathbb{N}$. Hence,

$$B_{\delta}(x) = \bigcup_{j \ge 1} A_j(x).$$

Now we can split the inner integral into layers according to these sets:

$$\begin{split} \int_{\partial D \cap B_{\delta}(x)} \frac{1}{|x - y|^{d-2}} \, dy &= \sum_{j \ge 1} \int_{\partial D \cap A_{j}(x)} \frac{1}{|x - y|^{d-2}} \, dy \\ &\leq \sum_{j \ge 1} \int_{\partial D \cap A_{j}(x)} \frac{1}{|2^{-j} \delta|^{d-2}} \, dy \\ &\leq \sum_{j \ge 1} 2^{j(d-2)} \delta^{2-d} |A_{j}(x)| \\ &= \delta^{2-d} \sum_{j \ge 1} 2^{j(d-2)} \Big[C \Big(2^{(1-j)d} \delta^{d} - 2^{-jd} \delta^{d} \Big) \Big] \\ &= \delta^{2} C \sum_{j \ge 1} 2^{j(d-2)-jd} \Big[2 - 1 \Big] = C \sum_{j \ge 1} \Big(\frac{1}{d} \Big)^{j} < \infty. \end{split}$$
(3.28)

Hence, combining (3.24) and (3.27) and using $|V|_{H^{\frac{1}{2}}(A)^d}^2 \leq |V|_{H^{\frac{1}{2}}(B)^d}^2$ for $A \subset B$, the result follows.

(3) The proof follows the lines of item (1) and is therefore left to the reader.

3.3 First-order asymptotic expansion

Let $u_0 \in H^1(\mathsf{D})^d$ denote the unique solution of the state equation (1.2) for $\varepsilon = 0$. We henceforth refer to u_0 as the unperturbed state variable. By definition u_0 satisfies $u_0|_{\Gamma} = u_D$ and

$$\int_{\mathsf{D}} \mathbf{C}_2 \boldsymbol{\epsilon}(u_0) : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \, dx = \int_{\mathsf{D}} f_2 \cdot \boldsymbol{\varphi} \, dx + \int_{\Gamma_N} u_N \cdot \boldsymbol{\varphi} \, dS \quad \text{for all } \boldsymbol{\varphi} \in H^1_{\Gamma}(\mathsf{D})^d. \tag{3.29}$$

Assumption 1. We henceforth assume that the $u_0 \in C^3(B_{\delta}(x_0))$ for a small radius $\delta > 0$. **Lemma 3.6.** There is a constant C > 0, such that for all $\varepsilon > 0$ sufficiently small there holds $\|u_{\varepsilon} - u_0\|_{H^1(\mathbb{D})^d} \leq C\varepsilon^{\frac{d}{2}}.$ (3.30)

Proof. Subtracting (3.1) for $\varepsilon > 0$ and (3.29) yields

$$\int_{\mathsf{D}} \mathbf{C}_{\omega_{\varepsilon}} \boldsymbol{\epsilon}(u_{\varepsilon} - u_0) : \boldsymbol{\epsilon}(\varphi) \, dx = \int_{\omega_{\varepsilon}} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(u_0) : \boldsymbol{\epsilon}(\varphi) \, dx \\ + \int_{\omega_{\varepsilon}} (f_1 - f_2) \cdot \varphi \, dx \quad \text{for all } \varphi \in H^1_{\Gamma}(\mathsf{D})^d.$$
(3.31)

Therefore, testing with $\varphi := u_{\varepsilon} - u_0 \in H^1_{\Gamma}(\mathsf{D})^d$, applying Korn's inequality to the gradient term on the left-hand side followed by Friedrich's inequality and using Hölder's inequality to estimate the right-hand side leads to

$$\|u_{\varepsilon} - u_{0}\|_{H^{1}(\mathbb{D})^{d}}^{2} \leq C \Big(\|(\mathbf{C}_{2} - \mathbf{C}_{1})\boldsymbol{\epsilon}(u_{0})\|_{L_{2}(\omega_{\varepsilon})^{d \times d}} + \|f_{1} - f_{2}\|_{L_{2}(\omega_{\varepsilon})^{d}} \Big) \|u_{\varepsilon} - u_{0}\|_{H^{1}(\mathbb{D})^{d}}, \quad (3.32)$$

for a positive constant C > 0. In view of Assumption 1, we have $u_0 \in C^3(B_{\delta}(x_0))$ for $\delta > 0$ small enough and thus (3.32) can be further estimated to obtain

$$\|u_{\varepsilon} - u_0\|_{H^1(\mathsf{D})^d} \le C\sqrt{\omega_{\varepsilon}} \Big(\|(\mathbf{C}_2 - \mathbf{C}_1)\boldsymbol{\epsilon}(u_0)\|_{C(\omega_{\varepsilon})^{d \times d}} + \|f_1 - f_2\|_{C(\omega_{\varepsilon})^d} \Big).$$
(3.33)

Now, the result follows from $\sqrt{|\omega_{\varepsilon}|} = \sqrt{|\omega|} \varepsilon^{\frac{d}{2}}$.

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Definition 3.7. For almost every $x \in D$, we define the first variation of the state u_{ε} by Adjoint-based

$$U_{\varepsilon}^{(1)}(x) := \left(\frac{u_{\varepsilon} - u_{0}}{\varepsilon}\right) \bigcirc \Phi_{\varepsilon}(x), \quad \varepsilon > 0.$$
(3.34) methods

The second variation of u_{ε} is defined by

$$U_{\varepsilon}^{(2)}(x) := \frac{U_{\varepsilon}^{(1)}(x) - U^{(1)}(x) - \varepsilon^{d-1} u^{(1)} \bigcirc \Phi_{\varepsilon}}{\varepsilon}, \quad \varepsilon > 0.$$
(3.35)

More generally, we define the *i*-th variation of u_{ε} for $i \ge 2$ by

$$U_{\varepsilon}^{(i+1)}(x) := \frac{U_{\varepsilon}^{(i)}(x) - U^{(i)}(x) - \varepsilon^{d-2} u^{(i)} \bigcirc \Phi_{\varepsilon}}{\varepsilon}, \quad \varepsilon > 0.$$
(3.36)

Here, $U^{(i)} : \mathbf{R}^d \to \mathbf{R}^d$ are so-called boundary layer correctors and $u^{(i)} : \mathbf{D} \to \mathbf{R}^d$ are regular correctors. The functions $U^{(i)}$ aim to approximate $U^{(i)}_{\varepsilon}$; however, they introduce an error at the boundary of D, which is corrected with the help of $u^{(i)}$.

By extending u_{ε} and u_0 outside of D by a continuous extension operator $E: H^1(\mathsf{D})^d \to H^1(\mathbf{R}^d)^d$, one can view $U_{\varepsilon}^{(1)}$ as an element of the Beppo-Levi space $BL(\mathbf{R}^d)^d$. In the following, we show that the first variation of the state converges to a function

In the following, we show that the first variation of the state converges to a function $U \in BL(\mathbf{R}^d)^d$ and determine an equation satisfied by this limit. The next Lemma helps us to handle the inhomogeneous Dirichlet boundary condition on Γ_{ε} .

Lemma 3.8. Let $A : \mathbf{R}^{d \times d} \to \mathbf{R}^{d \times d}$ be uniformly positive definite, $F_{\varepsilon} : H^{1}_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^{d} \to \mathbf{R}$ be a linear and continuous functional with respect to $\|\cdot\|_{\varepsilon}$ and $g_{\varepsilon} \in H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}$. Then there exists a unique $V_{\varepsilon} \in H^{1}(\mathsf{D}_{\varepsilon})^{d}$, such that

$$\int_{\mathsf{D}_{\varepsilon}} A\boldsymbol{\epsilon}(V_{\varepsilon}) : \boldsymbol{\epsilon}(\varphi) \, dx = F_{\varepsilon}(\varphi) \quad \text{for all } \varphi \in H^{1}_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^{d}, \tag{3.37}$$

$$V_{\varepsilon}|_{\Gamma_{\varepsilon}} = g_{\varepsilon}. \tag{3.38}$$

Furthermore, there exists a constant C > 0 such that

$$\|V_{\varepsilon}\|_{\varepsilon} \le C(\|F_{\varepsilon}\| + \varepsilon^{\frac{1}{2}}\|g_{\varepsilon}\|_{L_{2}(\Gamma_{\varepsilon})^{d}} + |g_{\varepsilon}|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}}).$$
(3.39)

Proof. Let $a_{\varepsilon}(u, v) := \int_{\mathsf{D}_{\varepsilon}} A\epsilon(u) : \epsilon(v) \, dx, \, u, v \in H^1(\mathsf{D}_{\varepsilon})^d$. Thanks to our assumption, A is uniformly positive definite and thus one readily checks that a_{ε} is an elliptic and continuous bilinear form on $H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d$ endowed with the scaled norm $\|\cdot\|_{\varepsilon}$. Furthermore, let $Z_{\Gamma_{\varepsilon}}$ denote the right-inverse extension operator of the trace operator $T_{\Gamma_{\varepsilon}}$ and define $G_{\varepsilon} := Z_{\Gamma_{\varepsilon}}(g_{\varepsilon}) \in H^1(\mathsf{D}_{\varepsilon})^d$.

Now consider
$$F_{\varepsilon}(\varphi) := F_{\varepsilon}(\varphi) - a_{\varepsilon}(G_{\varepsilon}, \varphi)$$
. Since

$$\tilde{F}_{\varepsilon}(\varphi) | \leq |F_{\varepsilon}(\varphi)| + |a_{\varepsilon}(G_{\varepsilon},\varphi)|
\leq C ||F_{\varepsilon}|| ||\varphi||_{\varepsilon} + C ||G_{\varepsilon}||_{\varepsilon} ||\varphi||_{\varepsilon} \leq C ||\varphi||_{\varepsilon} \quad \text{for all } \varphi \in H^{1}_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^{d},$$
(3.40)

for a constant C > 0, \tilde{F}_{ε} is continuous wih respect to $\|\cdot\|_{\varepsilon}$. Thus, by the Lax–Milgram theorem, there exists a unique $u_{\varepsilon} \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d$, such that

$$a_{\varepsilon}(u_{\varepsilon},\varphi) = \tilde{F}_{\varepsilon}(\varphi) \quad \text{for all } \varphi \in H^{1}_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^{d}.$$
(3.41)

Hence, we conclude that $V_{\varepsilon} := u_{\varepsilon} + G_{\varepsilon}$ satisfies (3.37) and (3.38). Uniqueness is guaranteed by the ellipticity of a_{ε} . Applying the triangle inequality and using the continuity of $Z_{\Gamma_{\varepsilon}}$ to estimate $\|G_{\varepsilon}\|_{\varepsilon}$ yields

$$\begin{split} \|V_{\varepsilon}\|_{\varepsilon} &\leq \|u_{\varepsilon}\|_{\varepsilon} + \|G_{\varepsilon}\|_{\varepsilon} \leq C\Big(\|\tilde{F}_{\varepsilon}\| + \|G_{\varepsilon}\|_{\varepsilon}\Big) \leq C\big(\|F_{\varepsilon}\| + \|G_{\varepsilon}\|_{\varepsilon}\Big) \\ &\leq C(\|F_{\varepsilon}\| + \varepsilon^{\frac{1}{2}}\|g_{\varepsilon}\|_{L_{2}(\Gamma_{\varepsilon})^{d}} + |g_{\varepsilon}|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}}), \end{split}$$

which shows (3.39) and finishes the proof.

Lemma 3.9. There exists a unique solution $[U] \in \dot{BL}(\mathbf{R}^d)^d$ to

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}([U]) : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \, dx \quad \text{for all } \boldsymbol{\varphi} \in \dot{BL}(\mathbf{R}^d)^d. \quad (3.42)$$

Moreover, there exists a representative $U^{(1)} \in [U]$, which satisfies pointwise for $|x| \to \infty$:

$$U^{(1)}(x) = R^{(1)}(x) + \mathcal{O}(|x|^{-d}), \qquad (3.43)$$

where $R^{(1)}: \mathbf{R}^d \to \mathbf{R}^d$ satisfies

$$|R^{(1)}(x)| = \begin{cases} b_2 |x|^{-1} & \text{for } d = 2, \\ b_3 |x|^{-2} & \text{for } d = 3, \end{cases}$$
(3.44)

for some constants $b_2, b_3 \in \mathbf{R}$.

Proof. Unique solvability of (3.42) follows directly from the Lemma of Lax–Milgram. Thus, the only thing left to show is the asymptotic behaviour (3.43) of $U^{(1)}$. For this we first note that $U^{(1)}$ can be characterised by the following set of equations:

$$-\operatorname{div}(\mathbf{C}_{1}\boldsymbol{\epsilon}(U^{(1)})) = 0 \qquad \text{in }\boldsymbol{\omega}, \tag{3.45}$$

$$-\operatorname{div}(\mathbf{C}_{2}\boldsymbol{\epsilon}(U^{(1)})) = 0 \qquad \text{in}\,\overline{\boldsymbol{\omega}}^{\mathsf{c}},\tag{3.46}$$

$$[U^{(1)}]^+ = [U^{(1)}]^-$$
 on $\partial \omega$, (3.47)

$$\left[\mathbf{C}_{1}\boldsymbol{\epsilon}(U^{(1)})\boldsymbol{n}\right]^{+} - \left[\mathbf{C}_{2}\boldsymbol{\epsilon}(U^{(1)})\boldsymbol{n}\right]^{-} = (\mathbf{C}_{2} - \mathbf{C}_{1})\boldsymbol{\epsilon}(U^{(1)})(\boldsymbol{x}_{0})\boldsymbol{n} \qquad \text{on } \partial\boldsymbol{\omega}.$$
(3.48)

By (Ammari, 2008, p. 76, Thm. 3.3.8) there are $f, g \in L_2(\partial \omega)^d$, such that

$$\begin{bmatrix} \mathcal{S}_{\omega}^{1}f \end{bmatrix}^{+} - \begin{bmatrix} \mathcal{S}_{\omega}^{2}g \end{bmatrix}^{-} = 0, \quad \text{on } \partial \omega$$

$$\begin{bmatrix} \mathbf{C}_{1}\boldsymbol{\epsilon}(\mathcal{S}_{\omega}^{1}f)n \end{bmatrix}^{+} - \begin{bmatrix} \mathbf{C}_{2}\boldsymbol{\epsilon}(\mathcal{S}_{\omega}^{2}g)n \end{bmatrix}^{-} = (\mathbf{C}_{2} - \mathbf{C}_{1})\boldsymbol{\epsilon}(U^{(1)})(x_{0})n, \quad \text{on } \partial \omega, \qquad (3.49)$$

where $S_{\omega}^{i}f$ denotes the single layer potential on $\partial \omega$ with respect to the fundamental solution Γ_{i} , that is, $S_{\omega}^{i}h(x) := \int_{\partial \omega} \Gamma_{i}(x-y)h(y) dS(y)$, $i \in \{1, 2\}$. Additionally, since $\int_{\partial \omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) \epsilon(U^{(1)})(x_{0})n dS = 0$, it follows that $\int_{\partial \omega} g dS = 0$. Thus,

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satisfies (3.45)–(3.48). Furthermore, considering $\int_{\partial \omega} g \, dS = 0$, a Taylor expansion of $\Gamma_2(x - y)$ in y = 0 yields the desired asymptotic behaviour (3.43).

 $U^{(1)} := \begin{cases} \mathcal{S}^{1}_{\omega} f & \text{in } \omega, \\ \mathcal{S}^{2}_{\omega} g & \text{in } \overline{\omega}^{\mathsf{c}}, \end{cases}$

Theorem 3.10. Let $U_{\varepsilon}^{(1)}$ be as in Definition 3.7 and $\alpha \in (0, 1)$. There exists a constant C > 0, such that

$$\|U_{\varepsilon}^{(1)} - U^{(1)}\|_{\varepsilon} \leq \begin{cases} C\varepsilon & \text{for } d = 3, \\ C\varepsilon^{1-\alpha} & \text{for } d = 2, \end{cases}$$
(3.50)

for ε sufficiently small.

Proof. We start by deriving an equation for $U_{\epsilon}^{(1)}$. For this purpose, we change variables in (3.31) to obtain

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon} \left(U_{\varepsilon}^{(1)} \right) : \boldsymbol{\epsilon}(\varphi) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(u_0) \circ \Phi_{\varepsilon} : \boldsymbol{\epsilon}(\varphi) \, dx + \boldsymbol{\varepsilon} \int_{\omega} (f_1 - f_2) \circ \Phi_{\varepsilon} \cdot \varphi \, dx \quad \text{for all } \varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d.$$
(3.51)

Splitting the integral on the left-hand side of (3.42), integrating by parts and using $\operatorname{Div}(\mathbf{C}_2 \in (U^{(1)})) = 0$ in $\overline{\omega}^c$ yields

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon} (U^{(1)}) : \boldsymbol{\epsilon} (\varphi) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon} (x_0) : \boldsymbol{\epsilon} (\varphi) \, dx - \int_{\mathbf{R}^d \setminus \mathsf{D}_{\varepsilon}} \mathbf{C}_2 \boldsymbol{\epsilon} (U^{(1)}) : \boldsymbol{\epsilon} (\tilde{\varphi}) \, dx$$

$$= \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon} (x_0) : \boldsymbol{\epsilon} (\varphi) \, dx - \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_2 \boldsymbol{\epsilon} (U^{(1)}) \tilde{n} \cdot \tilde{\varphi} \, dS$$

$$+ \int_{\mathbf{R}^d \setminus \mathsf{D}_{\varepsilon}} \operatorname{div} (\mathbf{C}_2 \boldsymbol{\epsilon} (U^{(1)})) \cdot \tilde{\varphi} \, dx$$

$$= \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon} (x_0) : \boldsymbol{\epsilon} (\varphi) \, dx + \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_2 \boldsymbol{\epsilon} (U^{(1)}) n \cdot \varphi \, dS,$$

$$(3.52)$$

where $\varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d$, $\tilde{\varphi}$ denotes an extension to the whole domain and \overline{n} denotes the outer normal vector on $\overline{D_{c}^{c}}$. Subtracting (3.51) and (3.52) results in

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon} \left(U_{\varepsilon}^{(1)} - U^{(1)} \right) : \boldsymbol{\epsilon}(\varphi) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) [\boldsymbol{\epsilon}(u_0) \circ \boldsymbol{\Phi}_{\varepsilon} - \boldsymbol{\epsilon}(u_0)(x_0)] : \boldsymbol{\epsilon}(\varphi) \, dx \\ + \boldsymbol{\epsilon} \int_{\omega} (f_1 - f_2) \circ \boldsymbol{\Phi}_{\varepsilon} \cdot \varphi \, dx \\ - \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_2 \boldsymbol{\epsilon} (U^{(1)}) n \cdot \varphi \, dS$$
(3.53)

for all $\varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d$. Now, we apply Lemma 3.8 to $V_{\varepsilon} := U_{\varepsilon}^{(1)} - U^{(1)}, g_{\varepsilon} := -U^{(1)}|_{\Gamma_{\varepsilon}}$ and F_{ε}^1 defined as the right-hand side of (3.53). Thus, we conclude that there exists a constant C > 0, such that

$$\|U_{\varepsilon}^{(1)} - U^{(1)}\|_{\varepsilon} \le C(\|F_{\varepsilon}^{1}\| + \varepsilon^{\frac{1}{2}}\|U^{(1)}\|_{L_{2}(\Gamma_{\varepsilon})^{d}} + |U^{(1)}|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}}).$$
(3.54)

To finish our proof, we need to estimate the norms of F_{ϵ}^{1} and $U^{(1)}$, which appear in (3.54). For the sake of clarity, we split the functional F_{ε}^1 according to (3.53) and treat each term separately. Let $\varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})$.

EC 39.1 (1) At first, we consider $\int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) [\epsilon(u_0) \circ \Phi_{\varepsilon} - \epsilon(u_0)(x_0)] : \epsilon(\varphi) \, dx$. Since $u_0 \in C^3(B_{\delta}(x_0))$, we get

$$\boldsymbol{\epsilon}(u_0)(x_0 + \boldsymbol{\epsilon} \boldsymbol{x}) = \boldsymbol{\epsilon}(u_0)(x_0) + \nabla \boldsymbol{\epsilon}(u_0)(x_0)\boldsymbol{\epsilon} \boldsymbol{x} + \boldsymbol{o}(\boldsymbol{\epsilon} \boldsymbol{x}). \tag{3.55}$$

Together with an application of Hölder's inequality, we conclude

$$\underbrace{\mathbf{80}} \qquad \left| \int_{\omega} [\boldsymbol{\epsilon}(u_0) \circ \boldsymbol{\Phi}_{\boldsymbol{\epsilon}} - \boldsymbol{\epsilon}(u_0)(x_0)] : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \, dx \right| \leq C \|\boldsymbol{\epsilon}(u_0) \circ \boldsymbol{\Phi}_{\boldsymbol{\epsilon}} - \boldsymbol{\epsilon}(u_0)(x_0)\|_{L_2(\omega)} \|\boldsymbol{\epsilon}(\boldsymbol{\varphi})\|_{L_2(\omega)^{d \times d}} \\ \leq C \boldsymbol{\epsilon} \|\boldsymbol{\epsilon}(\boldsymbol{\varphi})\|_{L_2(\omega)^{d \times d}} \leq C \boldsymbol{\epsilon} \|\boldsymbol{\varphi}\|_{\boldsymbol{\epsilon}}. \tag{3.56}$$

(2) Next, we consider $\varepsilon \int_{\omega} (f_1 - f_2) \circ \Phi_{\varepsilon} \cdot \varphi \, dx$. Since we want to apply the Gagliardo–Nirenberg inequality, we need to distinguish between dimensions d = 2 and d = 3.

For d = 3, an application of Hölder's inequality with respect to $p = 2^*$ and Lemma 3.4, item (2) yield

$$\left|\varepsilon \int_{\omega} (f_1 - f_2) \bigcirc \Phi_{\varepsilon} \cdot \varphi \, dx\right| \le C \varepsilon \|\varphi\|_{\varepsilon}. \tag{3.57}$$

For d = 2 we apply Hölder's inequality with respect to $p = (2 - \delta)^*$ for $\delta > 0$ sufficiently small and Lemma 3.4, item (3) to obtain

$$\left|\varepsilon \int_{\omega} (f_1 - f_2) \bigcirc \Phi_{\varepsilon} \cdot \varphi \, dx\right| \le C \varepsilon^{1-\alpha} \|\varphi\|_{\varepsilon}. \tag{3.58}$$

for a constant C > 0.

(3) Finally, the last term can be estimated using Hölder's inequality and the scaled trace inequality (Lemma 3.4 item (4)):

$$\left| \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2} \boldsymbol{\epsilon} (U^{(1)}) \boldsymbol{n} \cdot \boldsymbol{\varphi} \, dS \right| \leq C \left\| \boldsymbol{\epsilon} (U^{(1)}) \right\|_{L_{2}(\partial \mathsf{D}_{\varepsilon})^{d \times d}} \left\| \boldsymbol{\varphi} \right\|_{L_{2}(\partial \mathsf{D}_{\varepsilon})^{d}}$$
(3.59)

$$\leq C\varepsilon^{-\frac{1}{2}} \| \boldsymbol{\epsilon} (U^{(1)}) \|_{L_2(\partial \mathsf{D}_{\varepsilon})^{d \times d}} \| \boldsymbol{\varphi} \|_{\varepsilon}.$$
(3.60)

Thus, Lemma 3.5, item (3) with m = d - 1 yields

$$\left| \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_2 \epsilon (U^{(1)}) n \cdot \varphi \, dS \right| \le C \varepsilon^{\frac{d}{2}} \|\varphi\|_{\varepsilon}.$$
(3.61)

Combining these estimates results in

$$\|F_{\varepsilon}^{1}\| \leq \begin{cases} C\varepsilon & \text{for } d = 3, \\ C\varepsilon^{1-\alpha} & \text{for } d = 2, \end{cases}$$
(3.62)

for a constant C > 0. Furthermore, Lemma 3.5 item (1) and (2) with m = d - 1 yield

$$\|U^{(1)}\|_{L_2(\Gamma_{\varepsilon})^d} \le C\varepsilon^{\frac{d-1}{2}}, \quad |U^{(1)}|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^d} \le C\varepsilon^{\frac{d}{2}}.$$
(3.63)

Now plugging (3.62) and (3.63) into (3.54) finishes the proof.

Remark 3.11. Rewriting $U_{\varepsilon}^{1} - U^{1}$ leaves us with the first-order expansion Adjoint-based $u_{\varepsilon}(x) \approx u_0(x) + \varepsilon U^1 \big(\Phi_{\varepsilon}^{-1}(x) \big),$ methods

where

$$\|u_{\varepsilon} - [u_0 + \varepsilon U^1 \bigcirc \Phi_{\varepsilon}^{-1}]\|_{H^1(\mathbb{D})^d} = \begin{cases} \mathcal{O}\left(\varepsilon^{\frac{d}{2}+1}\right) & \text{for } d = 3, \\ \mathcal{O}\left(\varepsilon^{\frac{d}{2}+1-\alpha}\right) & \text{for } d = 2, \alpha > 0. \end{cases}$$
(3.64)

3.4 Second-order asymptotic expansion

3.4 Second-order asymptotic expansion As mentioned earlier, the boundary layer corrector $U^{(1)}$ introduces an error at the boundary of D. Therefore, we introduce the regular corrector $u^{(1)}$, which compensates the boundary error. Additionally, in order to obtain a second-order expansion, we introduce the second-order approximations $U^{(2)}$ and $u^{(2)}$. In contrast to the first-order approximation, we need to split the boundary layer corrector $U^{(2)}$ into two terms, where one solves a lower-order equation and the other solves an analogue to $U^{(1)}$. Furthermore, we need to add the regular corrector $u^{(2)}$ to compensate the error introduced by $U^{(2)}$. The following lemma describes each asymptotic expansion. each corrector:

Lemma 3.12.

(1) There is a unique solution $u^{(1)} \in H^1(\mathsf{D})^d$ with $u^{(1)}(x) = -R^{(1)}(x-x_0)$ on Γ , such that

$$\int_{\mathsf{D}} \mathbf{C}_2 \boldsymbol{\epsilon} \left(u^{(1)} \right) : \boldsymbol{\epsilon}(\varphi) \ dx = -\int_{\Gamma_N} \mathbf{C}_2 \boldsymbol{\epsilon} \left(R^{(1)} \right) (x - x_0) n \cdot \varphi \ dS, \tag{3.65}$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$.

(2) There is a solution
$$[U] \in \dot{BL}_{p}(\mathbf{R}^{d})^{d}$$
 to

$$\int_{\mathbf{R}^{d}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}([U]) : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \, dx = \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) [\nabla \boldsymbol{\epsilon}(u_{0})(x_{0})x] : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \, dx, \qquad (3.66)$$

for all $\varphi \in \dot{BL}_{b'}(\mathbf{R}^d)^d$, where

$$p = \begin{cases} 2+\delta & \text{for } d=2, \\ 2 & \text{for } d=3, \end{cases}$$

and $\delta > 0$ small. Moreover, there exists a representative $\widehat{U}^{(2)} \in [U]$, which satisfies pointwise for $|x| \to \infty$:

$$\widehat{U}^{(2)}(x) = \widehat{R}^{(2)}(x) + \mathcal{O}(|x|^{1-d}), \qquad (3.67)$$

where $\widehat{R}^{(2)}$: $\mathbf{R}^d \to \mathbf{R}^d$ satisfies

$$\widehat{R}^{(2)}(x)| = \begin{cases} \widehat{c}_2 \ln(|x|) & \text{for } d = 2, \\ \widehat{c}_3 |x|^{-1} & \text{for } d = 3, \end{cases}$$
(3.68)

for some constants $\hat{c}_2, \hat{c}_3 \in \mathbf{R}$.

EC 39,1 (3) There exists a solution $[U] \in \dot{BL}_{p}(\mathbf{R}^{d})^{d}$ to

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}([U]) : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \ dx = \int_{\omega} [(f_1(x_0) - f_2(x_0))] \cdot \boldsymbol{\varphi} \ dx, \tag{3.69}$$

for all $\varphi \in C_c^1(\mathbf{R}^d)^d$, where

$$p = \begin{cases} 2+\delta & \text{for } d=2, \\ 2 & \text{for } d=3, \end{cases}$$

and $\delta > 0$ small. Moreover, there exists a representative $\tilde{U}^{(2)} \in [U]$, which satisfies pointwise for $|x| \to \infty$:

$$\tilde{U}^{(2)}(x) = \tilde{R}^{(2)}(x) + \mathcal{O}(|x|^{1-d}), \qquad (3.70)$$

where $\tilde{R}^{(2)}$: $\mathbf{R}^d \rightarrow \mathbf{R}^d$ satisfies

$$\tilde{R}^{(2)}(x)| = \begin{cases} \tilde{c}_2 \ln(|x|) & \text{for } d = 2, \\ \tilde{c}_3 |x|^{-1} & \text{for } d = 3, \end{cases}$$
(3.71)

for some constants $\tilde{c}_2, \tilde{c}_3 \in \mathbf{R}$.

(4) There is a unique solution $u^{(2)} \in H^1(\mathsf{D})^d$ with $u^{(2)}(x) = -R^{(2)}(x - x_0)$ on Γ , such that

$$\int_{\mathsf{D}} \mathbf{C}_2 \boldsymbol{\epsilon} \left(u^{(2)} \right) : \boldsymbol{\epsilon}(\varphi) \ dx = -\int_{\Gamma_N} \mathbf{C}_2 \boldsymbol{\epsilon} \left(R^{(2)} \right) (x - x_0) n \cdot \varphi \ dS, \tag{3.72}$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$, where $R^{(2)} := \widehat{R}^{(2)} + \widetilde{R}^{(2)}$.

Remark 3.13. Note that the requirement for p to be greater than 2 in dimension two is necessary to guarantee that the gradient of $\tilde{U}^{(2)}$ and $\hat{U}^{(2)}$ is in $L_p(\mathbf{R}^d)^{d \times d}$, which is not true for p = 2. In fact, there is a solution $[U] \in \dot{BL}(\mathbf{R}^2)^2$ of (3.66), but no representative $U \in [U]$ has the desired asymptotic representation.

Proof. Unique solvability of (3.65) and (3.72) follows from the Lax–Milgram theorem. In order to show the existence and the desired representation formula of $\tilde{U}^{(2)}$, we use single layer potentials. Note that a solution $U \in BL_p(\mathbf{R}^d)^d$ of (3.69) can be characterised by the following set of equations:

$$-\operatorname{div}(\mathbf{C}_{1}\boldsymbol{\epsilon}(U)) = \left[\left(f_{1}(x_{0}) - f_{2}(x_{0}) \right) \right] \qquad \text{in }\boldsymbol{\omega}, \tag{3.73}$$

$$-\operatorname{div}(\mathbf{C}_{2}\boldsymbol{\epsilon}(U)) = 0 \qquad \text{ in } \overline{\boldsymbol{\omega}}^{\mathsf{c}}, \tag{3.74}$$

$$[U]^+ = [U]^- \qquad \text{on } \partial \omega, \tag{3.75}$$

$$\left[\mathbf{C}_{1}\boldsymbol{\epsilon}(U)\boldsymbol{n}\right]^{+} = \left[\mathbf{C}_{2}\boldsymbol{\epsilon}(U)\boldsymbol{n}\right]^{-} \qquad \text{on } \partial\boldsymbol{\omega}.$$
(3.76)

Now consider the volume potential $u(x) := \int_{\omega} \Gamma_1(x - y) [(f_1(x_0) - f_2(x_0))] dy$, for $x \in \omega$, which satisfies the inhomogeneous equation inside ω . By (Ammari, 2008, p. 76, Thm. 3.3.8) there are $f, g \in L_2(\partial \omega)^d$, such that.

$$\left[\mathcal{S}_{\omega}^{1}f\right]^{+} - \left[\mathcal{S}_{\omega}^{2}g\right]^{-} = -u|_{\partial\omega} \quad \text{on } \partial\omega, \tag{3.77} \quad \text{Adjoint-based} \\ \text{methods}$$

(3.78)

$$\left[\mathbf{C}_{1}\boldsymbol{\epsilon}\left(\boldsymbol{\mathcal{S}}_{\omega}^{1}\boldsymbol{f}\right)\boldsymbol{n}\right]^{+}-\left[\mathbf{C}_{2}\boldsymbol{\epsilon}\left(\boldsymbol{\mathcal{S}}_{\omega}^{2}\boldsymbol{g}\right)\boldsymbol{n}\right]^{-}=-\left(\mathbf{C}_{1}\boldsymbol{\epsilon}(\boldsymbol{u})\boldsymbol{n}\right)|_{\partial\boldsymbol{\omega}}\quad\text{ on }\partial\boldsymbol{\omega}.$$

Finally,

$$\tilde{\boldsymbol{U}}^{(2)} \coloneqq \begin{cases} \boldsymbol{u} + \mathcal{S}_{\boldsymbol{\omega}}^{1}\boldsymbol{f}, & \text{ in } \boldsymbol{\omega}, \\ \mathcal{S}_{\boldsymbol{\omega}}^{2}\boldsymbol{g}, & \text{ in } \overline{\boldsymbol{\omega}}^{c}. \end{cases}$$

satisfies (3.73)–(3.76) and a Taylor expansion of $S^2_{\omega}g$ shows the asymptotic representation of (3.70). The proof for $\hat{U}^{(2)}$ is similar and therefore omitted.

- **Remark 3.14.** As a consequence of the equivalence relation defining the Beppo-Levi space, the function $U^{(2)}$ is defined up to a constant. Thus, we are allowed to add arbitrary constants to the boundary layer corrector $U^{(2)}$. As a result of the additive property of the leading term $R^{(2)}(x) = \ln(x)$, we need to add the ε dependent constant $c \ln(\varepsilon)$, with a suitable constant $c \in \mathbf{R}$ in dimension d = 2. In dimension d = 3 this problem does not appear since the leading term $|x|^{-1}$ is multiplicative and therefore can be compensated by the factor ε^{d-2} found in Definition 3.7.
- **Remark 3.15.** A possible approach to approximate the solution $\tilde{U}^{(2)}$ of (3.69) numerically is to consider for each $\varepsilon > 0$ the unique solution $K_{\varepsilon} \in \overset{\bigcirc}{W_{b}^{1}}(\mathsf{D})^{d}$ satisfying

$$\varepsilon^2 \int_{\mathsf{D}} \mathbf{C}_{\omega_{\varepsilon}} \boldsymbol{\epsilon}(K_{\varepsilon}) : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \, dx = \int_{\omega_{\varepsilon}} [(f_1(x_0) - f_2(x_0))] \boldsymbol{\varphi} \, dx \tag{3.79}$$

for all $\varphi \in \overset{\circ}{W_{p}^{1}}(\mathsf{D})^{d}$. Applying Hölder's inequality and the Gagliardo–Nirenberg inequality, we get

$$\left| \int_{\omega_{\varepsilon}} \left[(f_1(x_0) - f_2(x_0)) \right] \varphi \, dx \right| \le |\omega_{\varepsilon}|^{\overline{\left((p')^* \right)'}} \| \nabla \varphi \|_{L_{p'}(\mathsf{D})^{d \times d}} \tag{3.80}$$

and thus follow

$$\varepsilon^{2} \| \nabla K_{\varepsilon} \|_{L_{p}(\mathbb{D})^{d \times d}} \leq C \varepsilon^{(p)} \quad ,$$

for a constant $C > 0$. Now a change of variables yields $\| \nabla (K_{\varepsilon} \odot \Phi_{\varepsilon}) \|_{L_{p}(\mathbb{D}_{\varepsilon})} \leq C$. Hence, $K_{\varepsilon} \circ \Phi_{\varepsilon}$

is bounded in \dot{BL}_p and therefore has a weakly convergent subsequent with limit [U] satisfying (3.69).

Theorem 3.16. Let $U_{\varepsilon}^{(2)}$ be as in Definition 3.7 and $\alpha \in (0, 1)$.

(1) There exists a constant C > 0, such that

$$\|U_{\varepsilon}^{(2)} - U^{(2)} - \varepsilon^{d-2} u^{(2)} \circ \Phi_{\varepsilon}(x)\|_{\varepsilon} \le C\varepsilon \qquad \text{for } d = 3, \tag{3.81}$$

$$\|U_{\varepsilon}^{(2)} - U^{(2)} - \varepsilon^{d-2}u^{(2)} \circ \Phi_{\varepsilon}(x) + c\ln(\varepsilon)\|_{\varepsilon} \le C\varepsilon^{1-\alpha} \qquad \text{for } d = 2,$$
(3.82)

for $\varepsilon > 0$ sufficiently small and a suitable constant $c \in \mathbf{R}$.

(2) For $d \in \{2, 3\}$, there holds $\lim_{\varepsilon \searrow 0} \|\varepsilon^{-1} (\nabla U_{\varepsilon}^{(1)} - \nabla U^{(1)}) - \nabla U^{(2)}\|_{L_{2}(\omega)^{d \times d}} = 0.$

Proof. ad (1): Similar to the estimation of the first-order expansion, we aim to apply Lemma 3.8 in order to handle the inhomogeneous Dirichlet boundary condition on Γ_{ε} . Hence, we start by deriving an equation satisfied by $U_{\varepsilon}^{(2)} - U^{(2)} - \varepsilon^{d-2}u^{(2)} \bigcirc \Phi_{\varepsilon}(x) = \varepsilon U_{\varepsilon}^{(3)}$. Dividing (3.53) by $\varepsilon > 0$, changing variables in (3.65) and (3.72) and integrating by parts in the exterior domain of (3.66) and (3.69) yield

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon} \left(\varepsilon U_{\varepsilon}^{(3)} \right) : \boldsymbol{\epsilon}(\boldsymbol{\varphi}) \, dx = F_{\varepsilon}^{2}(\boldsymbol{\varphi}) + F_{\varepsilon}^{3}(\boldsymbol{\varphi}), \quad \text{for all } \boldsymbol{\varphi} \in H_{\Gamma_{\varepsilon}}^{1}(\mathsf{D}_{\varepsilon}), \tag{3.83}$$

where

$$F_{\varepsilon}^{2} \coloneqq \int_{\omega} [(f_{1}(\Phi_{\varepsilon}(x)) - f_{2}(\Phi_{\varepsilon}(x))) - (f_{1}(x_{0}) - f_{2}(x_{0}))] \cdot \varphi \, dx + \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) [\varepsilon^{-1}(\epsilon(u_{0}) \odot \Phi_{\varepsilon} - \epsilon(u_{0})(x_{0})) - \nabla \epsilon(u_{0})(x_{0})x] : \epsilon(\varphi) \, dx$$
(3.84)
$$+ \varepsilon^{d-1} \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) [\epsilon(u^{(1)}(\Phi_{\varepsilon})) + \epsilon(u^{(2)}(\Phi_{\varepsilon}))] : \epsilon(\varphi) \, dx F_{\varepsilon}^{3} \coloneqq -\varepsilon^{-1} \int_{\Gamma_{N,\varepsilon}} [\mathbf{C}_{2}\epsilon(U^{(1)}) - \varepsilon^{d}\mathbf{C}_{2}\epsilon(R^{(1)})(\varepsilon x)] n \cdot \varphi \, dS - \int_{\Gamma_{N,\varepsilon}} [\mathbf{C}_{2}\epsilon(U^{(2)}) - \varepsilon^{d-1}\mathbf{C}_{2}\epsilon(R^{(2)})(\varepsilon x)] n \cdot \varphi \, dS.$$
(3.85)

Since the bilinear form only depends on the symmetrised gradient of $U_{\varepsilon}^{(3)}$, one readily checks that $\varepsilon U_{\varepsilon}^{(3)}+c\ln(\varepsilon)$ satisfies

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon} \left(\varepsilon U_{\varepsilon}^{(3)} + c \ln(\varepsilon) \right) : \boldsymbol{\epsilon}(\varphi) \, dx = F_{\varepsilon}^{2}(\varphi) + F_{\varepsilon}^{3}(\varphi), \quad \text{for all } \varphi \in H_{\Gamma_{\varepsilon}}^{1}(\mathsf{D}_{\varepsilon}). \tag{3.86}$$

Now we can apply Lemma 3.8 to

$$V_{\varepsilon} := \begin{cases} \varepsilon U_{\varepsilon}^{(3)} & \text{for } d = 3, \\ \varepsilon U_{\varepsilon}^{(3)} + c \ln(\varepsilon) & \text{for } d = 2, \end{cases}$$
$$F_{\varepsilon} := F_{\varepsilon}^{2} + F_{\varepsilon}^{3}$$

and

$$g_{\varepsilon} := \begin{cases} \left(\varepsilon^{d-2} R^{(1)}(\varepsilon x) - \varepsilon^{-1} U^{(1)} \right)|_{\Gamma_{\varepsilon}} + \left(\varepsilon^{d-2} R^{(2)}(\varepsilon x) - U^{(2)} \right)|_{\Gamma_{\varepsilon}} & \text{for } d = 3, \\ \left(\varepsilon^{d-2} R^{(1)}(\varepsilon x) - \varepsilon^{-1} U^{(1)} \right)|_{\Gamma_{\varepsilon}} + \left(\varepsilon^{d-2} R^{(2)}(\varepsilon x) - U^{(2)} + c \ln(\varepsilon) \right)|_{\Gamma_{\varepsilon}} & \text{for } d = 2. \end{cases}$$
(3.87)

Hence, we get the apriori estimate

$$\|V_{\varepsilon}\|_{\varepsilon} \leq C(\|F_{\varepsilon}\| + \varepsilon^{\frac{1}{2}} \|g_{\varepsilon}\|_{L_{2}(\Gamma_{\varepsilon})^{d}} + |g_{\varepsilon}|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}}).$$

$$(3.88)$$

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EC 39,1 Due to great similarity between d = 2 and d = 3, we will discuss both cases together and only highlight the terms that have to be treated separately. Thus, if not further specified, let d = 2, 3. Again, we start by estimating $||F_{\varepsilon}||$. Let $\varphi \in H^{1}_{\Gamma_{\varepsilon}}(D_{\varepsilon})$.

(1) A Taylor expansion of $(f_1(\Phi_{\varepsilon}(x)) - f_2(\Phi_{\varepsilon}(x)))$ at x_0 , Hölder's inequality and Lemma 3.4, item (2), (3) yield

$$\left| \int_{\omega} \left[(f_1(\Phi_{\varepsilon}(x)) - f_2(\Phi_{\varepsilon}(x))) - (f_1(x_0) - f_2(x_0)) \right] \cdot \varphi \, dx \right| \le \begin{cases} C\varepsilon \|\varphi\|_{\varepsilon} & \text{for } d = 3, \\ C\varepsilon^{1-\alpha} \|\varphi\|_{\varepsilon} & \text{for } d = 2, \alpha > 0, \end{cases}$$

$$(3.89)$$

for a constant C > 0.

(2) Since u_0 is three times differentiable in a neighbourhood of x_0 , there is a constant C > 0, such that $|\varepsilon^{-1}(\epsilon(u_0) \circ \Phi_{\varepsilon} - \epsilon(u_0)(x_0)) - \nabla \epsilon(u_0)(x_0)x| \le C\varepsilon$, for $x \in \omega$. Hence, Hölder's inequality yields

$$\left| \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \left[\varepsilon^{-1}(\boldsymbol{\epsilon}(u_0) \circ \boldsymbol{\Phi}_{\varepsilon} - \boldsymbol{\epsilon}(u_0)(x_0)) - \nabla \varepsilon(u_0)(x_0)x \right] : \boldsymbol{\epsilon}(\varphi) \, dx \right| \leq C \varepsilon \|\varphi\|_{\varepsilon}.$$
(3.90)

(3) Furthermore, by Hölder's inequality we get

$$\left|\varepsilon^{d-1} \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \left[\epsilon \left(u^{(1)}(\Phi_{\varepsilon}) \right) + \epsilon \left(u^{(2)}(\Phi_{\varepsilon}) \right) \right] : \epsilon(\varphi) \, dx \right| \le C \varepsilon \|\varphi\|_{\varepsilon}, \qquad (3.91)$$

for a constant C > 0.

Next we consider the boundary integral terms:

(4) Here, we note that ϵ(U⁽¹⁾) − ε^dϵ(R⁽¹⁾)(εx) cancels out the leading term of U⁽¹⁾ on ∂D. Thus, we can apply Hölder's inequality, Lemma 3.5, item (3) with m = d and the scaled trace inequality to conclude

$$\left| \varepsilon^{-1} \int_{\Gamma_{N,\varepsilon}} \left[\mathbf{C}_{2} \boldsymbol{\epsilon} \left(U^{(1)} \right) - \varepsilon^{d} \mathbf{C}_{2} \boldsymbol{\epsilon} \left(R^{(1)} \right) (\varepsilon x) \right] n \cdot \boldsymbol{\varphi} \, dS \right| \leq C \varepsilon^{\frac{d}{2}} \| \boldsymbol{\varphi} \|_{\varepsilon}, \tag{3.92}$$

for a constant C > 0.

(5) Similarly, we deduce from Lemma 3.5, item (3) with m = d - 1 that there is a constant C > 0, such that

$$\left| \int_{\Gamma_{N,\varepsilon}} \left[\mathbf{C}_{2} \boldsymbol{\epsilon} \left(U^{(2)} \right) - \boldsymbol{\varepsilon}^{d-1} \mathbf{C}_{2} \boldsymbol{\epsilon} \left(R^{(2)} \right) (\boldsymbol{\varepsilon} \boldsymbol{x}) \right] \boldsymbol{n} \cdot \boldsymbol{\varphi} \, dS \right| \leq C \boldsymbol{\varepsilon}^{\frac{d}{2}} \| \boldsymbol{\varphi} \|_{\varepsilon}. \tag{3.93}$$

Combining the previous estimates yields

$$\|F_{\varepsilon}\| \le \begin{cases} C\varepsilon & \text{for } d = 3, \\ C\varepsilon^{1-\alpha} & \text{for } d = 2, \end{cases}$$
(3.94)

for a constant C > 0. Finally, we recall that g_{ε} is defined in (3.87). At this point we choose the constant $c \in \mathbf{R}$, such that

$$R^{(2)}(x) = R^{(2)}(\varepsilon x) + c\ln(\varepsilon) \quad \text{in } d = 2.$$

Then, by Lemma 3.5, item (1), (2) with m = d and m = d - 1 respectively, there is a constant C > 0, such that

$$\varepsilon^{\frac{1}{2}} \|g_{\varepsilon}\|_{L_{2}(\Gamma_{\varepsilon})^{d}} + \|g_{\varepsilon}\|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}} \le C\varepsilon^{\frac{d}{2}}.$$
(3.95)

Now we can plug (3.94) and (3.95) into the a priori estimate (3.88), which shows (3.81). ad (2): By the triangle inequality, we have

$$\begin{aligned} \|\varepsilon^{-1} \Big(\nabla \Big(U_{\varepsilon}^{(1)} \Big) - \nabla \big(U^{(1)} \big) \Big) - \nabla \big(U^{(2)} \big) \|_{L_{2}(\omega)^{d \times d}} &\leq \|\nabla \Big(U_{\varepsilon}^{(2)} - U^{(2)} - \varepsilon^{d-2} u^{(2)} \circ \Phi_{\varepsilon} \Big) \|_{L_{2}(\omega)^{d \times d}} \\ &+ \varepsilon^{d-1} \|\nabla \big(u^{(1)} \big) \circ \Phi_{\varepsilon} \|_{L_{2}(\omega)^{d \times d}} + \varepsilon^{d-1} \|\nabla \big(u^{(2)} \big) \circ \Phi_{\varepsilon} \|_{L_{2}(\omega)^{d \times d}} \leq C \varepsilon^{1-\alpha}, \end{aligned}$$

$$(3.96)$$

for a positive constant C. This shows (2) and therefore finishes the proof.

Remark 3.17. Note that by the triangle inequality one has

$$\begin{split} \|\varepsilon^{-1} \Big(U_{\varepsilon}^{(1)} - U^{(1)} \Big) - U^{(2)} \|_{\varepsilon} &\leq \left\| U_{\varepsilon}^{(2)} - U^{(2)} - \varepsilon^{d-2} u^{(2)} \bigcirc \Phi_{\varepsilon}(x) \right\|_{\varepsilon} + \left\| \varepsilon^{d-2} u^{(1)} \oslash \Phi_{\varepsilon}(x) \right\|_{\varepsilon} \\ &+ \left\| \varepsilon^{d-2} u^{(2)} \bigcirc \Phi_{\varepsilon}(x) \right\|_{\varepsilon} \\ &\leq C \Big(\varepsilon + \varepsilon^{\frac{1}{2}} \Big), \end{split}$$

for d = 3 and a constant C > 0. Thus in dimension d = 3, the correction of $u^{(2)}$ is not necessary to achieve convergence of $U_{\varepsilon}^{(2)}$. In fact, sparing the corrector results in a slower convergence of order $\varepsilon^{\frac{1}{2}}$ compared to the corrected order ε .

Remark 3.18. In order to give a better understanding of the scheme of the asymptotic expansion, we would like to point out the main difference between the firstand second-order expansion, which is the slower decay of the boundary layer corrector $U^{(2)}$ compared to $U^{(1)}$. As a result, there was no necessity to introduce the regular corrector $u^{(1)}$ in the first-order expansion, whereas $u^{(2)}$ was needed to obtain the desired order of at least $\varepsilon^{1-\alpha}$, for $\alpha > 0$ small. Additionally, one should note that boundary layer correctors appearing in higher-order expansions have asymptotics similar to $U^{(2)}$ and therefore demand a correction of the associated regular correctors. Thus, the scheme of the asymptotic expansion of arbitrary order resembles the second-order expansion given in this chapter, rather than the first-order expansion.

4. Analysis of the perturbed adjoint equation

In this section we study the asymptotic analysis of the Amstutz' adjoint equation and the averaged adjoint equation for our elasticity model problem. We shall first exam Amstutz' adjoint and derive its asymptotic expansion up to order two.

4.1 Amstutz' adjoint equation

The adjoint state $p_{\varepsilon}, \varepsilon \geq 0$ satisfies

$$p_{\varepsilon} \in H^{1}_{\Gamma}(\mathsf{D})^{a}, \quad \partial_{u} \mathcal{L}(\varepsilon, u_{0}, p_{\varepsilon})(\varphi) = 0 \quad \text{for all } \varphi \in H^{1}_{\Gamma}(\mathsf{D})^{a}, \tag{4.1}$$

where we recall the Lagrangian

$$\mathcal{L}(\varepsilon, u, v) = J_{\varepsilon}(u) + a_{\varepsilon}(u, v) - f_{\varepsilon}(v).$$
(4.2)

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With the cost function defined in (1.1), this equation reads explicitly

 $\int_{\mathsf{D}} \mathbf{C}_{\omega_{\varepsilon}} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(\boldsymbol{p}_{\varepsilon}) \, d\boldsymbol{x} = -\gamma_{f} \int_{\mathsf{D}} f_{\omega_{\varepsilon}} \cdot \boldsymbol{\varphi} \, d\boldsymbol{x} - 2\gamma_{m} \int_{\Gamma_{m}} (u_{0} - u_{m}) \cdot \boldsymbol{\varphi} \, dS$ $-2\gamma_{g} \int_{\mathsf{D}} [\nabla u_{0} - \nabla u_{d}] : \nabla \boldsymbol{\varphi} \, d\boldsymbol{x},$ (4.3)

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$. Similarly, the unperturbed adjoint equation reads

$$\int_{\mathsf{D}} \mathbf{C}_{2} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(\boldsymbol{p}_{0}) \, d\boldsymbol{x} = -\gamma_{f} \int_{\mathsf{D}} f_{2} \cdot \boldsymbol{\varphi} \, d\boldsymbol{x} - 2\gamma_{m} \int_{\Gamma_{m}} (u_{0} - u_{m}) \cdot \boldsymbol{\varphi} \, dS -2\gamma_{g} \int_{\mathsf{D}} [\nabla u_{0} - \nabla u_{d}] : \nabla \boldsymbol{\varphi} \, d\boldsymbol{x},$$

$$(4.4)$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$. Note that the ε dependence of p_{ε} is only via the coefficients $\mathbf{C}_{\omega_{\varepsilon}}$ and $f_{\omega_{\varepsilon}}$. This is a definite advantage over the averaged adjoint method, where also the perturbed state variable u_{ε} appears.

We now compute an asymptotic expansion of p_{ε} in a similar fashion to the direct state u_{ε} . Therefore we define the variation of the adjoint state $P_{\varepsilon}^{(i)}$ for $i \ge 1$ in analogy to the definition of the variation of the direct state (Definition 3.7), where we replace the boundary layer correctors $U^{(i)}$ by similar correctors $P^{(i)}$ adapted to the new inhomogeneity and the regular correctors $u^{(i)}$ are replaced by correctors $p^{(i)}$ matching $P^{(i)}$.

Lemma 4.1. There exists a solution $[P] \in \dot{BL}(\mathbf{R}^d)^d$ to

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}([P]) \ dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(p_0)(x_0) \ dx, \tag{4.5}$$

for all $\varphi \in \dot{BL}(\mathbf{R}^d)^d$. Moreover, there exists a representative $P^{(1)} \in [P]$, which satisfies pointwise for $|x| \to \infty$:

$$P^{(1)}(x) = S^{(1)}(x) + \mathcal{O}\left(|x|^{-d}\right), \tag{4.6}$$

where $S^{(1)}: \mathbf{R}^d \to \mathbf{R}^d$ satisfies

$$|S^{(1)}(x)| = \begin{cases} b_2 |x|^{-1} & \text{for } d = 2, \\ b_3 |x|^{-2} & \text{for } d = 3, \end{cases}$$
(4.7)

for some constants $b_2, b_3 \in \mathbf{R}$.

Proof. Using the adjoint tensor $\mathbf{C}_{\omega}^{\top} : \mathbf{R}^{d \times d} \to \mathbf{R}^{d \times d}$, we can rewrite (4.5) to get

$$\int_{\mathbf{R}^d} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \mathbf{C}_{\boldsymbol{\omega}}^\top \boldsymbol{\epsilon}([P]) \ d\boldsymbol{x} = \int_{\boldsymbol{\omega}} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \left(\mathbf{C}_2^\top - \mathbf{C}_1^\top\right) \boldsymbol{\epsilon}(p_0)(x_0) \ d\boldsymbol{x}.$$
(4.8)

Thus, using single layer potentials, the proof follows the lines of Lemma 3.9. \Box

Theorem 4.2. For $\alpha \in (0, 1)$ and $\varepsilon > 0$ sufficiently small there is a constant C > 0, such that

$$\|P_{\varepsilon}^{(1)} - P^{(1)}\|_{\varepsilon} \leq \begin{cases} C\varepsilon & \text{for } d = 3, \\ C\varepsilon^{1-\alpha} & \text{for } d = 2. \end{cases}$$

$$(4.9)$$

Proof. Similarly to the analysis of the direct state, we derive an equation of the form

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon} \left(P_{\varepsilon}^{(1)} - P^{(1)} \right) \, dx = G_{\varepsilon}^{1}(\boldsymbol{\varphi}) \quad \text{for all } \boldsymbol{\varphi} \in H_{\Gamma_{\varepsilon}}^{1}(\mathsf{D}_{\varepsilon})^{d}, \tag{4.10}$$

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where the right-hand side satisfies

$$\|G_{\varepsilon}^{1}\| \leq \begin{cases} C\varepsilon & \text{for } d = 3, \\ C\varepsilon^{1-\alpha} & \text{for } d = 2. \end{cases}$$

$$(4.11)$$

A detailed derivation and estimation of the functional G_{ε}^{1} can be found in the Appendix (Section A1). In view of Lemma 3.8, we now estimate the boundary integral terms. Since $P_{\varepsilon}^{(1)}|_{\Gamma_{\varepsilon}} = 0$ we follow from Lemma 3.5 item (1), (2) with m = d - 1 that there is a constant C > 0, such that

$$\varepsilon^{\frac{1}{2}} \| P_{\varepsilon}^{(1)} - P^{(1)} \|_{L_{2}(\Gamma_{\varepsilon})^{d}} + | P_{\varepsilon}^{(1)} - P^{(1)} |_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}} \le C \varepsilon^{\frac{d}{2}}.$$
(4.12)

Thus, considering (4.11) and (4.12), an application of Lemma 3.8 with $A = \mathbf{C}_{\omega}^{\top}$ shows (4.9), which finishes our proof.

We now continue with the second-order expansion. Similar to the state variable expansion, we therefore introduce a number of correctors in the following Lemma, which approximate the first-order expansion inside ω_{e} and on the boundary ∂D respectively.

Lemma 4.3.

(1) There is a unique solution $p^{(1)} \in H^1(\mathsf{D})^d$ with $p^{(1)}(x) = -S^{(1)}(x - x_0)$ on Γ , such that

$$\int_{\mathsf{D}} \mathbf{C}_2 \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(\boldsymbol{p}^{(1)}) = -\int_{\Gamma_N} \mathbf{C}_2^\top \boldsymbol{\epsilon}(S^{(1)})(\boldsymbol{x} - \boldsymbol{x}_0) \boldsymbol{n} \cdot \boldsymbol{\varphi} \, dS, \tag{4.13}$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$.

(2) There is a solution $[P] \in \dot{BL}_{p}(\mathbf{R}^{d})^{d}$ to

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}([P]) \ dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : [\nabla \boldsymbol{\epsilon}(\boldsymbol{p}_0)(\boldsymbol{x}_0) \boldsymbol{x}] \ dx, \tag{4.14}$$

for all $\varphi \in \dot{BL}_{p'}(\mathbf{R}^d)^d$, where

$$p = \begin{cases} 2+\delta & \text{for } d=2, \\ 2 & \text{for } d=3, \end{cases}$$

and $\delta > 0$ small. Moreover, there exists a representative $\widehat{P}^{(2)} \in [P]$, which satisfies pointwise for $|x| \to \infty$:

$$\widehat{P}^{(2)}(x) = \widehat{S}^{(2)}(x) + \mathcal{O}(|x|^{1-d}),$$
(4.15)

where $\widehat{S}^{(2)} : \mathbf{R}^d \to \mathbf{R}^d$ satisfies

$$|\widehat{S}^{(2)}(x)| = \begin{cases} \widehat{c}_2 \ln(|x|) & \text{for } d = 2, \\ \widehat{c}_3 |x|^{-1} & \text{for } d = 3, \end{cases}$$
(4.16)

for some constants $\hat{c}_2, \hat{c}_3 \in \mathbf{R}$.

(3) There is a solution $[P] \in \dot{BL}_{p}(\mathbf{R}^{d})^{d}$ to

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}([P]) \ dx = \gamma_f \int_{\omega} [f_2(x_0) - f_1(x_0)] \cdot \boldsymbol{\varphi} \ dx, \tag{4.17}$$

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for all $\varphi \in C_c^1(\mathbf{R}^d)^d$, where

 $p = \begin{cases} 2+\delta & \text{for } d=2, \\ 2 & \text{for } d=3, \end{cases}$

and $\delta > 0$ small. Moreover, there exists a representative $\tilde{P}^{(2)} \in [P]$, which satisfies pointwise for $|x| \to \infty$:

$$\tilde{P}^{(2)}(x) = \tilde{S}^{(2)}(x) + \mathcal{O}(|x|^{1-d}),$$
(4.18)

where $\tilde{S}^{(2)} : \mathbf{R}^d \to \mathbf{R}^d$ satisfies

$$|\tilde{S}^{(2)}(x)| = \begin{cases} \tilde{c}_2 \ln(|x|) & \text{for } d = 2, \\ \tilde{c}_3 |x|^{-1} & \text{for } d = 3, \end{cases}$$
(4.19)

for some constants $\tilde{c}_2, \tilde{c}_3 \in \mathbf{R}$.

(4) There is a unique solution
$$p^{(2)} \in H^1(\mathsf{D})^d$$
 with $p^{(2)}(x) = -S^{(2)}(x-x_0)$ on Γ , such that

$$\int_{\mathsf{D}} \mathbf{C}_{2} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(\boldsymbol{p}^{(2)}) = -\int_{\Gamma_{N}} \mathbf{C}_{2}^{\top} \boldsymbol{\varepsilon}(S^{(2)}) (\boldsymbol{x} - \boldsymbol{x}_{0}) \boldsymbol{n} \cdot \boldsymbol{\varphi} \, dS \tag{4.20}$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$, where $S^{(2)} := \widehat{S}^{(2)} + \widetilde{S}^{(2)}$.

Proof. Rewriting these equations with the help of the adjoint operator $\mathbf{C}_{\omega}^{\top}$ leads to a proof similar to Lemma 3.12.

Now we are able to state our main result regarding the second-order expansion of the adjoint state variable p_{e} :

Theorem 4.4.

(1) There exists a constant C > 0, such that

$$\|P_{\varepsilon}^{(2)} - P^{(2)} - \varepsilon^{d-2} p^{(2)} \circ \Phi_{\varepsilon}\|_{\varepsilon} \le C\varepsilon \qquad \text{for } d = 3, \tag{4.21}$$

$$\|P_{\varepsilon}^{(2)} - P^{(2)} - \varepsilon^{d-2} p^{(2)} \circ \Phi_{\varepsilon} + c \ln(\varepsilon)\|_{\varepsilon} \le C \varepsilon^{1-\alpha} \qquad \text{for } d = 2,$$
(4.22)

for ε sufficiently small and a suitable constant $c \in \mathbf{R}$.

(2) For
$$d \in \{2, 3\}$$
, there holds $\lim_{\varepsilon \searrow 0} \|\varepsilon^{-1}(\nabla(P_{\varepsilon}^{(1)}) - \nabla(P^{(1)})) - \nabla(P^{(2)})\|_{L_2(\omega)^{d \times d}} = 0.$

Proof. ad (1): For the sake of clarity, we restrict ourselves to the case of d = 3. Dimension d = 2 can be treated in a similar fashion. In view of the auxiliary result Lemma 3.8, we seek a governing equation for $\varepsilon P_{\varepsilon}^{(3)} = P_{\varepsilon}^{(2)} - P^{(2)} - \varepsilon^{d-2} p^{(2)} \bigcirc \Phi_{\varepsilon}$. Such an equation can be found using similar techniques to the analysis of the direct state. Thus, we refer to the Appendix (Section A2) for more details regarding the exact computation and only mention that there are functionals G_{ε}^2 , G_{ε}^3 , such that

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon} \left(\varepsilon P_{\varepsilon}^{(3)} \right) dx = G_{\varepsilon}^{2}(\varphi) + G_{\varepsilon}^{3}(\varphi) \quad \text{for all } \varphi \in H_{\Gamma_{\varepsilon}}^{1}(\mathsf{D}_{\varepsilon})^{d}, \tag{4.23}$$

where G_{ε}^{k} , k = 2, 3, satisfy

$$\|G_{\varepsilon}^{k}\| \le C\varepsilon, \tag{4.24}$$

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for $k \in \{2, 3\}$ and a constant C > 0. The exact formulas of the functionals G_e^2 , G_e^3 can be found in the Appendix (Section A2). Since

$$\varepsilon P_{\varepsilon}^{(3)}|_{\Gamma_{\varepsilon}} = \left(\varepsilon^{d-2}S^{(1)}(\varepsilon x) - \varepsilon^{-1}P^{(1)}\right)|_{\Gamma_{\varepsilon}} + \left(\varepsilon^{d-2}S^{(2)}(\varepsilon x) - P^{(2)}\right)|_{\Gamma_{\varepsilon}},$$

it follows by Lemma 3.5 item (1), (2) with m = d - 1 and m = d respectively that

 $\varepsilon^{\frac{1}{2}} \| \varepsilon P_{\varepsilon}^{(3)} \|_{L_2(\Gamma_{\varepsilon})^d} + | \varepsilon P_{\varepsilon}^{(3)} |_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^d} \le C \varepsilon^{\frac{d}{2}}.$ (4.25)

Hence, considering (4.24) and (4.25), Lemma 3.8 shows (4.21).

ad (2): By the triangle inequality we have

$$\begin{aligned} \|\varepsilon^{-1} \Big(\nabla \Big(P_{\varepsilon}^{(1)} \Big) - \nabla \big(P^{(1)} \big) \Big) - \nabla \big(P^{(2)} \big) \|_{L_{2}(\omega)^{d \times d}} \\ & \leq \Big\| \nabla \Big(P_{\varepsilon}^{(2)} - P^{(2)} - \varepsilon^{d-2} p^{(2)} \bigcirc \Phi_{\varepsilon} \Big) \|_{L_{2}(\omega)^{d \times d}} \\ & + \varepsilon^{d-1} \Big\| \nabla \big(p^{(1)} \big) \odot \Phi_{\varepsilon} \|_{L_{2}(\omega)^{d \times d}} + \varepsilon^{d-1} \Big\| \nabla \big(p^{(2)} \big) \odot \Phi_{\varepsilon} \|_{L_{2}(\omega)^{d \times d}} \\ & \leq C \varepsilon^{1-\alpha}, \end{aligned}$$

$$(4.26)$$

for a positive constant *C*. This shows (2) and therefore finishes the proof.

4.2 Averaged adjoint equation

The averaged adjoint state q_{ε} satisfies

$$q_{\varepsilon} \in H^{1}_{\Gamma}(\mathsf{D})^{d}, \quad a_{\varepsilon}(\varphi, q_{\varepsilon}) = -\int_{0}^{1} \partial J_{\varepsilon}(su_{\varepsilon} + (1 - s)u_{0})(\varphi) \, ds \quad \text{for all } \varphi \in H^{1}_{\Gamma}(\mathsf{D})^{d}.$$
(4.27)

With the cost function defined in (1.1), this equation reads explicitly

$$\int_{\mathsf{D}} \mathbf{C}_{\omega_{\varepsilon}} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(q_{\varepsilon}) \, dx = -\gamma_m \int_{\Gamma_m} (u_0 + u_{\varepsilon} - 2u_m) \cdot \boldsymbol{\varphi} \, dS - \gamma_f \int_{\mathsf{D}} f_{\omega_{\varepsilon}} \cdot \boldsymbol{\varphi} \, dx - \gamma_g \int_{\mathsf{D}} [\nabla u_0 + \nabla u_{\varepsilon} - 2\nabla u_d] : \nabla \boldsymbol{\varphi} \, dx,$$
(4.28)

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$. Similarly, the unperturbed adjoint equation reads

$$\int_{\mathsf{D}} \mathbf{C}_{2} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(q_{0}) \, dx = -2\gamma_{m} \int_{\Gamma_{m}} (u_{0} - u_{m}) \cdot \boldsymbol{\varphi} \, dS - \gamma_{f} \int_{\mathsf{D}} f_{2} \cdot \boldsymbol{\varphi} \, dx -2\gamma_{g} \int_{\mathsf{D}} [\nabla u_{0} - \nabla u_{d}] : \nabla \boldsymbol{\varphi} \, dx,$$

$$(4.29)$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$. Considering (4.4), we would like to point out that p_0 and q_0 satisfy the same equation and due to unique solvability it follows $p_0 = q_0$. Note that for the sake of simplicity we have chosen $\gamma_g = \gamma_m = 0$ in d = 2, as these terms lead to a more complicated analysis of the asymptotic expansion of q_g .

We now introduce the first terms of the asymptotic expansion:

Lemma 4.5.

(1) There exists a solution $[Q] \in \dot{BL}(\mathbf{R}^d)^d$ to $\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon}([Q]) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon}(q_0)(x_0) \, dx, \tag{4.30}$ for all $\varphi \in BL(\mathbf{R}^d)^d$. Moreover, there exists a representative $\widehat{Q}^{(1)} \in [Q]$, which satisfies Adjoint-based methods

$$\widehat{Q}^{(1)}(x) = \widehat{T}^{(1)}(x) + \mathcal{O}(|x|^{-d}),$$
(4.31)

where $\widehat{\boldsymbol{T}}^{(1)}: \mathbf{R}^d \rightarrow \mathbf{R}^d$ satisfies

$$|\widehat{T}^{(1)}(x)| = \begin{cases} \widehat{b}_2 |x|^{-1} & \text{for } d = 2, \\ \widehat{b}_3 |x|^{-2} & \text{for } d = 3, \end{cases}$$
(4.32)

for some constants $\hat{b}_2, \hat{b}_3 \in \mathbf{R}$.

(2) There exists a solution $[Q] \in \dot{BL}(\mathbf{R}^3)^3$ to

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}([Q]) \ dx = -\gamma_g \int_{\mathbf{R}^d} \nabla U^{(1)} : \nabla \boldsymbol{\varphi} \ dx, \tag{4.33}$$

for all $\varphi \in \dot{BL}(\mathbb{R}^3)^3$. Moreover, there exists a representative $\tilde{Q}^{(1)} \in [Q]$, which satisfies pointwise for $|x| \to \infty$:

$$\tilde{Q}^{(1)}(x) = \tilde{T}^{(1)}(x) + \mathcal{O}\Big(\ln(|x|)|x|^{-2}\Big), \tag{4.34}$$

where $\tilde{T}^{(1)} : \mathbf{R}^d \to \mathbf{R}^d$ satisfies

$$|\tilde{T}^{(1)}(x)| = \tilde{b}_3 |x|^{-1} \tag{4.35}$$

for a constant $\tilde{b}_3 \in \mathbf{R}$. Now let

$$Q^{(1)} := \begin{cases} \widehat{Q}^{(1)} + \widetilde{Q}^{(1)} & \text{for } d = 3, \\ \widehat{Q}^{(1)} & \text{for } d = 2, \end{cases}$$

and similarly

$$T^{(1)} := \begin{cases} \hat{T}^{(1)} + \tilde{T}^{(1)} & \text{for } d = 3, \\ \hat{T}^{(1)} & \text{for } d = 2. \end{cases}$$

Proof. Similar to Lemma 4.1, but due to the inhomogeneity in the exterior domain, we use a Newton potential to represent the solution. \Box

Theorem 4.6. For $\alpha \in (0, 1)$ and $\varepsilon > 0$ sufficiently small there is a constant C > 0, such that

$$\|Q_{\varepsilon}^{(1)} - Q^{(1)}\|_{\varepsilon} \leq \begin{cases} C\varepsilon^{\frac{1}{2}} & \text{for } d = 3, \\ C\varepsilon^{1-\alpha} & \text{for } d = 2. \end{cases}$$

$$(4.36)$$

Proof. We only show the case of d = 3, since the proof for d = 2 follows the same lines. Again, we start by deriving an equation of the form

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon} \left(Q_{\varepsilon}^{(1)} - Q^{(1)} \right) \, d\boldsymbol{x} = G_{\varepsilon}^{4}(\boldsymbol{\varphi}), \tag{4.37}$$

for all $\varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d$, where

$$\|G_{\varepsilon}^4\| \le C\varepsilon^{\frac{1}{2}}.\tag{4.38}$$

 \square

A detailed derivation and estimation of the functional G_{ε}^4 can be found in the Appendix (Section A3). In view of Lemma 3.8 we now estimate the boundary integral terms. Since $Q_{\varepsilon}^{(1)}|_{\Gamma_{\varepsilon}} = 0$ we deduce from Lemma 3.5 item (1), (2) with m = d - 1 that there is a constant C > 0 satisfying

$$\varepsilon^{\frac{1}{2}} \|Q_{\varepsilon}^{(1)} - Q^{(1)}\|_{L_{2}(\Gamma_{\varepsilon})^{d}} + |Q_{\varepsilon}^{(1)} - Q^{(1)}|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^{d}} \le C\varepsilon^{\frac{1}{2}}.$$
(4.39)

Thus, considering (4.38) and (4.39), an application of Lemma 3.8 shows (4.36).

We now continue with the second-order expansion. Similar to the previous asymptotic expansions, we therefore introduce each component in the following lemma. Note that the regular correctors aim to approximate $U^{(1)}$ in addition to their approximation of the occurring boundary layer correctors $Q^{(1)}$, $Q^{(2)}$. This is a result of the appearance of $U_{\varepsilon}^{(1)}$ on the right-hand side of (4.37), (A.17).

Lemma 4.7.

(1) There is a unique solution $q^{(1)} \in H^1(\mathsf{D})^d$ with $q^{(1)}(x) = -T^{(1)}(x-x_0)$ on Γ , such that

$$\int_{\mathsf{D}} \mathbf{C}_{2} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(\boldsymbol{q}^{(1)}) \ d\boldsymbol{x} = -\int_{\Gamma_{N}} \mathbf{C}_{2}^{\top} \boldsymbol{\epsilon}(\boldsymbol{T}^{(1)}) (\boldsymbol{x} - \boldsymbol{x}_{0}) \boldsymbol{n} \cdot \boldsymbol{\varphi} \ d\boldsymbol{S}, \tag{4.40}$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$.

(2) There is a solution $[Q] \in \dot{BL}_{b}(\mathbf{R}^{d})^{d}$ to

$$\int_{\mathbf{R}^{d}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}([Q]) \, d\boldsymbol{x} = \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : [\nabla \boldsymbol{\epsilon}(q_{0})(x_{0})\boldsymbol{x}] \, d\boldsymbol{x} - \gamma_{g} \int_{\mathbf{R}^{d}} \nabla U^{(2)} : \nabla \boldsymbol{\varphi} \, d\boldsymbol{x},$$
(4.41)

for all $\varphi \in \dot{BL}_{p'}(\mathbf{R}^d)^d$, where

$$p = \begin{cases} 2+\delta & \text{for } d=2, \\ 2 & \text{for } d=3, \end{cases}$$

and $\delta > 0$ small. Moreover, there exists a representative $\widehat{Q}^{(2)} \in [Q]$, which satisfies pointwise for $|x| \to \infty$:

$$\widehat{Q}^{(2)}(x) = \widehat{T}^{(2)}(x) + \begin{cases} \mathcal{O}(|x|^{-1}) & \text{for } d = 2, \\ \mathcal{O}(\ln(|x|)|x|^{-2}) & \text{for } d = 3, \end{cases}$$
(4.42)

where $\widehat{T}^{(2)}$: $\mathbf{R}^d \to \mathbf{R}^d$ satisfies

$$|\widehat{T}^{(2)}(x)| = \begin{cases} \widehat{c}_2 \ln(|x|) & \text{for } d = 2, \\ \widehat{c}_3 \ln(|x|) |x|^{-1} & \text{for } d = 3, \end{cases}$$
(4.43)

for some constants $\hat{c}_2, \hat{c}_3 \in \mathbf{R}$.

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EC 39,1 (3) There is a solution $[Q] \in \dot{BL}_{p}(\mathbf{R}^{d})^{d}$ to

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon}([Q]) \ dx = \gamma_f \int_{\omega} [f_2(x_0) - f_1(x_0)] \cdot \varphi \ dx, \tag{4.44}$$
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for all $\varphi \in C_c^1(\mathbf{R}^d)^d$, where

$$p = \begin{cases} 2+\delta & \text{for } d=2, \\ 2 & \text{for } d=3, \end{cases}$$
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and $\delta > 0$ small. Moreover, there exists a representative $\tilde{Q}^{(2)} \in [Q]$, which satisfies pointwise for $|x| \to \infty$:

$$\tilde{P}^{(2)}(x) = \tilde{T}^{(2)}(x) + \mathcal{O}(|x|^{1-d}),$$
(4.45)

where $\tilde{T}^{(2)}: \mathbf{R}^d \to \mathbf{R}^d$ satisfies

$$|\tilde{T}^{(2)}(x)| = \begin{cases} \tilde{c}_2 \ln(|x|) & \text{for } d = 2, \\ \tilde{c}_3 |x|^{-1} & \text{for } d = 3, \end{cases}$$
(4.46)

for some constants $\tilde{c}_2, \tilde{c}_3 \in \mathbf{R}$.

(4) There is a unique solution $q_U^{(2)} \in H^1_{\Gamma}(\mathsf{D})^d$, such that

$$\int_{D} \mathbf{C}_{2} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}\left(\boldsymbol{q}_{U}^{(2)}\right) d\boldsymbol{x} = -\gamma_{m} \int_{\Gamma_{m}} R^{(1)} (\boldsymbol{x} - \boldsymbol{x}_{0}) \cdot \boldsymbol{\varphi} \, d\boldsymbol{S} - \gamma_{m} \int_{\Gamma_{m}} \boldsymbol{u}^{(1)} \cdot \boldsymbol{\varphi} \, d\boldsymbol{S}$$
$$-\gamma_{m} \int_{\Gamma_{m}} R^{(2)} (\boldsymbol{x} - \boldsymbol{x}_{0}) \cdot d\boldsymbol{S} - \gamma_{m} \int_{\Gamma_{m}} \boldsymbol{u}^{(2)} \cdot \boldsymbol{\varphi} \, d\boldsymbol{S}$$
$$-\gamma_{g} \int_{D} \nabla \boldsymbol{u}^{(1)} : \nabla \boldsymbol{\varphi} \, d\boldsymbol{x} - \gamma_{g} \int_{D} \nabla \boldsymbol{u}^{(2)} : \nabla \boldsymbol{\varphi} \, d\boldsymbol{x}$$
$$-\gamma_{g} \int_{\Gamma_{N}} \nabla R^{(1)} (\boldsymbol{x} - \boldsymbol{x}_{0}) \boldsymbol{n} \cdot \boldsymbol{\varphi} \, d\boldsymbol{S}$$
$$-\gamma_{g} \int_{\Gamma_{N}} \nabla R^{(2)} (\boldsymbol{x} - \boldsymbol{x}_{0}) \boldsymbol{n} \cdot \boldsymbol{\varphi} \, d\boldsymbol{S}$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$.

(5) There is a unique solution $q_Q^{(2)} \in H^1(\mathsf{D})^d$ with $q^{(2)}(x) = -T^{(2)}(x-x_0)$ on Γ , such that

$$\int_{\mathsf{D}} \mathbf{C}_{2} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon} \left(q_{Q}^{(2)} \right) \, dx = -\int_{\Gamma_{N}} \mathbf{C}_{2}^{\top} \, \boldsymbol{\epsilon} \left(T^{(2)} \right) (x - x_{0}) n \cdot \boldsymbol{\varphi} \, dS \tag{4.48}$$

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$, where

$$T^{(2)} := \begin{cases} \widehat{T}^{(2)} + \widetilde{T}^{(2)} & \text{for } d = 2, \\ \widehat{T}^{(2)} & \text{for } d = 3. \end{cases}$$

Furthermore, we define $q^{(2)}\!:=\!q_U^{(2)}+q_Q^{(2)}.$

Proof. Similar to Lemma 3.12 and Lemma 4.5.

Now we are able to state our main result regarding the second-order expansion of the averaged adjoint state variable q_{ε} :

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Theorem 4.8.

(1) Let $\alpha \in (0, 1)$. There exists a constant C > 0, such that for d = 3 and d = 2, we have respectively:

$$\|\varepsilon^{-1} \Big[Q_{\varepsilon}^{(1)} - Q^{(1)} - \varepsilon^{d-2} q^{(1)} \bigcirc \Phi_{\varepsilon} \Big] - Q^{(2)} - \varepsilon^{d-2} q^{(2)} \bigcirc \Phi_{\varepsilon} \|_{\varepsilon} \leq C \varepsilon^{\frac{1}{2}} \ln(\varepsilon^{-1})$$
(4.49)

$$\left\|\varepsilon^{-1}\left[Q_{\varepsilon}^{(1)}-Q^{(1)}-\varepsilon^{d-1}q^{(1)}\bigcirc\Phi_{\varepsilon}\right]-Q^{(2)}-\varepsilon^{d-2}q^{(2)}\bigcirc\Phi_{\varepsilon}+c\ln(\varepsilon)\right\|_{\varepsilon} \leq C\varepsilon^{1-\alpha} \quad (4.50)$$

for ε sufficiently small and a suitable constant $c \in \mathbf{R}$.

(2) For $d \in \{2, 3\}$, there holds $\lim_{\varepsilon \to 0} \|\varepsilon^{-1} (\nabla Q_{\varepsilon}^{(1)} - \nabla Q^{(1)}) - \nabla Q^{(2)}\|_{L_2(\omega)^{d \times d}} = 0.$

Proof. ad (1): Similar to the proof of the second-order expansion of the adjoint state variable, we restrict ourselves to the case of d = 3. The proof for dimension d = 2 follows the same lines and is therefore omitted. In view of the auxiliary result Lemma 3.8, we seek a governing equation for $V_{\varepsilon} := \varepsilon^{-1}[Q_{\varepsilon}^{(1)} - Q^{(1)}] - \varepsilon^{d-3}q^{(1)} \bigcirc \Phi_{\varepsilon} - Q^{(2)} - \varepsilon^{d-2}q^{(2)} \bigcirc \Phi_{\varepsilon}$. Such an equation can be found using similar techniques to the analysis of the direct state and the derivation will be discussed in detail in the Appendix (see Section A4). We just note that there are functionals $G_{\varepsilon}^5, G_{\varepsilon}^6$ such that

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon}(V_{\varepsilon}) \, dx = G_{\varepsilon}^{5}(\varphi) + G_{\varepsilon}^{6}(\varphi) \quad \text{for all } \varphi \in H^{1}_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^{d}, \tag{4.51}$$

where G_{ϵ}^{k} , k = 5, 6, satisfy

$$\|G_{\varepsilon}^{k}\| \le C\varepsilon^{\frac{1}{2}}\ln(\varepsilon^{-1}), \tag{4.52}$$

for $k \in \{5, 6\}$ and a constant C > 0. The exact formulas of the functionals G_{e}^{5} , G_{e}^{6} can be found in the Appendix (Section A4). Since

$$V_{arepsilon}|_{\Gamma_{arepsilon}} = ig(arepsilon^{d-2}T^{(1)}(arepsilon x) - arepsilon^{-1}Q^{(1)}ig)|_{\Gamma_{arepsilon}} - Q^{(2)}|_{\Gamma_{arepsilon}}$$

it follows with a similar argument to Lemma 3.5 that there is a constant C > 0 satisfying

$$\varepsilon^{\frac{1}{2}} \| V_{\varepsilon} \|_{L_2(\Gamma_{\varepsilon})^d} + \| V_{\varepsilon} \|_{H^{\frac{1}{2}}(\Gamma_{\varepsilon})^d} \le C \varepsilon^{\frac{1}{2}} \ln(\varepsilon^{-1}).$$

$$(4.53)$$

In view of (4.52) and (4.53), Lemma 3.8 shows (4.49).

ad (2): Let d = 3. By the triangle inequality we have

$$\begin{aligned} \|\varepsilon^{-1} \left(\nabla \left(Q_{\varepsilon}^{(1)} \right) - \nabla \left(Q^{(1)} \right) \right) - \nabla \left(Q^{(2)} \right) \|_{L_{2}(\omega)^{d \times d}} \\ & \leq \left\| \varepsilon^{-1} \nabla \left(Q_{\varepsilon}^{(1)} - Q^{(1)} \right) - \nabla \left(\varepsilon^{d-3} q^{(1)} \odot \Phi_{\varepsilon} \right) - \nabla \left(\varepsilon^{d-2} q^{(2)} \odot \Phi_{\varepsilon} \right) \|_{L_{2}(\omega)^{d \times d}} \\ & + \varepsilon^{d-2} \left\| \nabla \left(q^{(1)} \right) \odot \Phi_{\varepsilon} \right\|_{L_{2}(\omega)^{d \times d}} + \varepsilon^{d-1} \left\| \nabla \left(q^{(2)} \right) \odot \Phi_{\varepsilon} \right\|_{L_{2}(\omega)^{d \times d}} \\ & \leq C \varepsilon^{\frac{1}{2}} \ln(\varepsilon^{-1}), \end{aligned}$$

$$(4.54)$$

for a positive constant *C*, which shows (2). The proof for d = 2 follows the same lines and is therefore omitted.

5. Computation of the topological derivatives for linear elasticity problem In this section we compute the first- and second-order topological derivatives of our elasticity problem introduced in (1.1), namely

$$\mathcal{J}(\mathbf{\Omega}) = J(\mathbf{\Omega}, u) = \gamma_m \int_{\Gamma_m} |u - u_m|^2 \, dS + \gamma_f \int_{\mathsf{D}} f_{\omega_e} \cdot u \, dx + \gamma_g \int_{\mathsf{D}} |\nabla u - \nabla u_d|^2 \, dx, \qquad (5.1)$$

subject to $u \in H^1(\mathsf{D})^d$ solves $u|_{\Gamma} = u_D$ and

$$\int_{\mathsf{D}} \mathbf{C}_{\Omega} \boldsymbol{\epsilon}(u) : \boldsymbol{\epsilon}(\varphi) = \int_{\mathsf{D}} f_{\Omega} \cdot \varphi \, dx + \int_{\Gamma_N} u_N \cdot \varphi \, dS \quad \text{for all } \varphi \in H^1_{\Gamma}(\mathsf{D})^d.$$
(5.2)

Definition 5.1. For $\varepsilon \ge 0$ let $\Omega_{\varepsilon} \subset D$ be a singularly perturbed domain with perturbation shape ω and $\Omega := \Omega_0$. Additionally let $\ell_1, \ell_2 : \mathbf{R}^+ \to \mathbf{R}^+$ be two functions converging to 0 for $\varepsilon \searrow 0$ and $\frac{\ell_1(\varepsilon)}{\ell_2(\varepsilon)} \to 0$ for $\varepsilon \searrow 0$. Then the first-order topological derivative is defined as

$$d\mathcal{J}(\mathbf{\Omega},\omega) = \lim_{arepsilon \searrow 0} rac{\mathcal{J}(\mathbf{\Omega}_arepsilon) - \mathcal{J}(\mathbf{\Omega})}{\ell_1(arepsilon)}$$

Similarly, the second-order topological derivative is given as

$$d^2 \mathcal{J}(\Omega,\omega) = \lim_{\epsilon \searrow 0} rac{\mathcal{J}(\Omega_\epsilon) - \mathcal{J}(\Omega) - \ell_1(\epsilon) d\mathcal{J}(\Omega)}{\ell_2(\epsilon)}.$$

More specifically, since we considered $\Omega = \emptyset$, we compute the topological derivative at a point $x_0 \in D$ and derive the asymptotics of $\mathcal{J}(\omega_{\varepsilon})$ with $\omega_{\varepsilon} := \Phi_{\varepsilon}(\omega)$, $\Phi_{\varepsilon}(x) := x_0 + \varepsilon x$. Recall the Lagrangian function

$$\mathcal{L}(\varepsilon, u, v) = J_{\varepsilon}(u) + a_{\varepsilon}(u, v) - f_{\varepsilon}(v), \quad u \in \mathcal{V}, \ v \in \mathcal{W},$$

with $\mathcal{V} = \{u \in H^1(\mathsf{D})^d | u = u_D \text{ on } \Gamma\}, \mathcal{W} = H^1_{\Gamma}(\mathsf{D})^d \text{ and }$

$$J_{\varepsilon}(u) = \gamma_m \int_{\Gamma_m} |u - u_m|^2 \, dS + \gamma_f \int_{\mathsf{D}} f_{\omega_{\varepsilon}} \cdot u \, dx + \gamma_g \int_{\mathsf{D}} |\nabla u - \nabla u_d|^2 \, dx, \tag{5.3}$$

$$a_{\varepsilon}(u,v) = \int_{\mathsf{D}} \mathbf{C}_{\omega_{\varepsilon}} \boldsymbol{\epsilon}(u) : \boldsymbol{\epsilon}(v) \, dx, \qquad (5.4)$$

$$f_{\varepsilon}(v) = \int_{\mathsf{D}} f_{\omega_{\varepsilon}} \cdot v \, dx. \tag{5.5}$$

We compute the topological derivatives using Proposition 2.2 (Amstutz' method), Proposition 2.4 (averaged adjoint) and Proposition 2.7 (Delfour's method).

Remark 5.2. We would like to point out that, contrary to the setting in Section 2, \mathcal{V} is a affine space spanned by \mathcal{W} and not a vector space itself. Yet, it can easily be verified that the Lagrangian techniques can still be applied, as the

construction of \mathcal{V} allows derivatives of $\mathcal{L}(\varepsilon, u, v)$ with respect to the second variable in direction \mathcal{W} .

Remark 5.3. Note that the more general case $\Omega \neq \emptyset$, $x_0 \in D \setminus \overline{\Omega}$ and $\Omega_{\varepsilon} = \Omega \cup \omega_{\varepsilon}$ can be treated in a similar fashion. The main difference is that the unperturbed state equation and unperturbed adjoint state equation respectively depend on Ω and therefore u_0 and p_0 vary. Furthermore, as the boundary layer correctors coincide in both cases, the regular correctors need to compensate in Ω . At last, the computation of the topological derivative for $x_0 \in \Omega$ and $\Omega_{\varepsilon} = \Omega \setminus \omega_{\varepsilon}$ can be done analogously to the presented one and only results in a change of sign.

5.1 Amstutz' method

In order to compute the first-order topological derivative, let $\ell_1(\varepsilon) := |\omega_{\varepsilon}|$. By Proposition 2.2, item (1), we have

$$d\mathcal{J}(\emptyset,\omega)(x_0) = \mathcal{R}^{(1)}(u_0,p_0) + \partial_{\ell}^{(1)}\mathcal{L}(0,u_0,p_0),$$
(5.6)

where

$$\mathcal{R}^{(1)}(u_0, p_0) = \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_\varepsilon, p_\varepsilon) - \mathcal{L}(\varepsilon, u_0, p_\varepsilon)}{\ell_1(\varepsilon)},$$
(5.7)

$$\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0) = \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_0, p_{\varepsilon}) - \mathcal{L}(0, u_0, p_{\varepsilon})}{\ell_1(\varepsilon)},$$
(5.8)

if the above limits exist. Thus, we start with the first quotient $\mathcal{R}^{(1)}(u_0, p_0)$:

$$\frac{\mathcal{L}(\varepsilon, u_{\varepsilon}, p_{\varepsilon}) - \mathcal{L}(\varepsilon, u_{0}, p_{\varepsilon})}{\ell_{1}(\varepsilon)} = \frac{1}{|\omega_{\varepsilon}|} [J_{\varepsilon}(u_{\varepsilon}) + a_{\varepsilon}(u_{\varepsilon}, p_{\varepsilon}) - f_{\varepsilon}(p_{\varepsilon}) - J_{\varepsilon}(u_{0}) - a_{\varepsilon}(u_{0}, p_{\varepsilon}) + f_{\varepsilon}(p_{\varepsilon})] \\
= \frac{1}{|\omega_{\varepsilon}|} [J_{\varepsilon}(u_{\varepsilon}) - J_{\varepsilon}(u_{0}) + a_{\varepsilon}(u_{\varepsilon} - u_{0}, p_{\varepsilon})] \\
= \frac{1}{|\omega_{\varepsilon}|} \gamma_{m} \int_{\Gamma_{m}} [|u_{\varepsilon} - u_{m}|^{2} - |u_{0} - u_{m}|^{2} - 2(u_{0} - u_{m})(u_{\varepsilon} - u_{0})] dS \\
+ \frac{1}{|\omega_{\varepsilon}|} \gamma_{g} \int_{D} [|\nabla u_{\varepsilon} - \nabla u_{d}|^{2} - |\nabla u_{0} - \nabla u_{d}|^{2} - 2(\nabla u_{0} - \nabla u_{d})(\nabla u_{\varepsilon} - \nabla u_{0})] dx \\
= \frac{1}{|\omega_{\varepsilon}|} \gamma_{m} \int_{\Gamma_{m}} |u_{\varepsilon} - u_{0}|^{2} dS + \frac{1}{|\omega_{\varepsilon}|} \gamma_{g} \int_{D} |\nabla u_{\varepsilon} - \nabla u_{0}|^{2} dx.$$
(5.9)

Now, a change of variables leads to $\frac{\varepsilon}{|\omega|} \gamma_m \|U_{\varepsilon}^{(1)}\|_{L_2(\Gamma_{m,\varepsilon})^d}^2 + \frac{1}{|\omega|} \gamma_g \|\nabla U_{\varepsilon}^{(1)}\|_{L_2(\mathsf{D}_{\varepsilon})^{d \times d}}^2$. On the one hand, we have

$$\frac{\varepsilon}{|\omega|} \gamma_m \|U_{\varepsilon}^{(1)}\|_{L_2(\Gamma_{m,\varepsilon})^d}^2 \leq \frac{\gamma_m}{|\omega|} \left(\varepsilon \|U_{\varepsilon}^{(1)} - U^{(1)}\|_{L_2(\Gamma_{m,\varepsilon})^d}^2 + \varepsilon \|U^{(1)}\|_{L_2(\Gamma_{m,\varepsilon})^d}^2\right) \\
\leq C \left(\|U_{\varepsilon}^{(1)} - U^{(1)}\|_{\varepsilon}^2 + \varepsilon^d\right) \leq C\varepsilon^{2-\alpha},$$
(5.10)

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for α arbitrarily small and a constant C > 0. Here, we used Lemma 3.4, item (4), Lemma 3.5 item (1) with m = d - 1 and Theorem 3.10. On the other hand, Theorem 3.10 shows that $\nabla U_{\varepsilon}^{(1)} \rightarrow \nabla U^{(1)}$ in $L_2(\mathbf{R}^d)^{d \times d}$ for $\varepsilon \searrow 0$. Now, passing to the limit in (5.9) yields Adjoint-based methods

$$\mathcal{R}^{(1)}(u_0, p_0) = \frac{1}{|\omega|} \gamma_g \int_{\mathbf{R}^d} |\nabla U^{(1)}|^2 dx.$$

Next, we consider $\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0)$. Splitting the quotient, one observes

$$\frac{\mathcal{L}(\varepsilon, u_{0}, p_{\varepsilon}) - \mathcal{L}(0, u_{0}, p_{\varepsilon})}{\ell_{1}(\varepsilon)} = \frac{1}{|\omega_{\varepsilon}|} [J_{\varepsilon}(u_{0}) + a_{\varepsilon}(u_{0}, p_{\varepsilon}) - f_{\varepsilon}(p_{\varepsilon}) - J_{0}(u_{0}) - a_{0}(u_{0}, p_{\varepsilon}) + f_{0}(p_{\varepsilon})] \\
= \frac{1}{|\omega_{\varepsilon}|} \int_{\omega_{\varepsilon}} [\gamma_{f}(f_{1} - f_{2})u_{0} + (\mathbf{C}_{1} - \mathbf{C}_{2})\epsilon(u_{0}) : \epsilon(p_{\varepsilon}) - (f_{1} - f_{2})p_{\varepsilon}] dx \\
= \gamma_{f} \int_{\omega} (f_{1} \circ \Phi_{\varepsilon} - f_{2} \circ \Phi_{\varepsilon}) \cdot u_{0} \circ \Phi_{\varepsilon} dx \\
+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})\epsilon(u_{0}) \circ \Phi_{\varepsilon} : \epsilon(p_{\varepsilon}^{(1)}) dx \tag{5.11} \\
+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})\epsilon(u_{0}) \circ \Phi_{\varepsilon} : \epsilon(p_{0}) \circ \Phi_{\varepsilon} dx \\
- \int_{\omega} (f_{1} \circ \Phi_{\varepsilon} - f_{2} \circ \Phi_{\varepsilon}) \cdot (P_{\varepsilon}^{(1)}) dx \\
- \int_{\omega} (f_{1} \circ \Phi_{\varepsilon} - f_{2} \circ \Phi_{\varepsilon}) \cdot p_{0} \circ \Phi_{\varepsilon} dx.$$

By Hölder's inequality, Lemma 3.4, item (2), (3) and Theorem 4.6 one readily checks that $P_{\varepsilon}^{(1)} \rightarrow P^{(1)}$ in $L_1(\omega)^d$ and $\epsilon(Q_{\varepsilon}^{(1)}) \rightarrow \epsilon(Q^{(1)})$ in $L_2(\omega)^{d \times d}$. Hence, we deduce

$$\begin{aligned}
\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0) &= \int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(P^{(1)}) \, dx \\
&+ \gamma_f(f_1(x_0) - f_2(x_0)) \cdot u_0(x_0) \\
&+ (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(p_0)(x_0) \\
&- (f_1(x_0) - f_2(x_0)) \cdot p_0(x_0).
\end{aligned}$$
(5.12)

Therefore, the first-order topological derivative is given by

$$d\mathcal{J}(\emptyset,\omega)(x_0) = \int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(P^{(1)}) \, dx + (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(p_0)(x_0) + \gamma_f(f_1(x_0) - f_2(x_0)) \cdot u_0(x_0) - (f_1(x_0) - f_2(x_0)) \cdot p_0(x_0) + \frac{1}{|\omega|} \gamma_g \int_{\mathbf{R}^d} |\nabla U^{(1)}|^2 \, dx,$$
(5.13)

with $P^{(1)}$ defined in (4.5) and $U^{(1)}$ defined in (3.42). Next, we compute the second-order topological derivative. Therefore, let $\ell_2(\varepsilon) := \varepsilon \ell_1(\varepsilon)$. By Proposition 2.2, item (2), we have

$$d^{2}\mathcal{J}(\emptyset,\omega)(x_{0}) = \mathcal{R}^{(2)}(u_{0},p_{0}) + \partial_{\ell}^{(2)}\mathcal{L}(0,u_{0},p_{0}),$$
(5.14)

where

$$\frac{\text{EC}}{39,1} \qquad \qquad \mathcal{R}^{(2)}(u_0,p_0) = \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon,u_\varepsilon,p_\varepsilon) - \mathcal{L}(\varepsilon,u_0,p_\varepsilon) - \ell_1(\varepsilon)\mathcal{R}^{(1)}(u_0,p_0)}{\ell_2(\varepsilon)}$$

$$\partial_{\ell}^{(2)}\mathcal{L}(0, u_0, p_0) = \lim_{\varepsilon \searrow 0} \frac{\mathcal{L}(\varepsilon, u_0, p_{\varepsilon}) - \mathcal{L}(0, u_0, p_{\varepsilon}) - \ell_1(\varepsilon)\partial_{\ell}^{(2)}\mathcal{L}(0, u_0, p_0)}{\ell_2(\varepsilon)}$$

if the above limits exist. Dividing (5.9) by ε , it follows that

$$\mathcal{R}^{(2)}(u_{0},p_{0}) = \lim_{\varepsilon \searrow 0} \frac{\gamma_{g}}{\varepsilon} \left[\int_{\mathsf{D}_{\varepsilon}} |\nabla U_{\varepsilon}^{(1)}|^{2} - |\nabla U^{(1)}|^{2} dx - \int_{\mathbf{R}^{d} \backslash \mathsf{D}_{\varepsilon}} |\nabla U^{(1)}|^{2} dx \right]$$

$$= \lim_{\varepsilon \searrow 0} \gamma_{g} \left[\int_{\mathsf{D}_{\varepsilon}} \left(U_{\varepsilon}^{(1)} + U^{(1)} \right) : \left(\varepsilon^{-1} \left[U_{\varepsilon}^{(1)} - U^{(1)} \right] \right) dx - \varepsilon^{-1} \int_{\mathbf{R}^{d} \backslash \mathsf{D}_{\varepsilon}} |\nabla U^{(1)}|^{2} dx \right] \quad (5.15)$$

$$= 2\gamma_{g} \frac{1}{|\omega|} \int_{\mathbf{R}^{d}} \nabla U^{(1)} : \nabla U^{(2)} dx,$$

where we used that $\nabla U_{\varepsilon}^{(1)} \to \nabla U^{(1)}$ in $L_2(\mathbf{R}^d)^{d \times d}$ (see Theorem 3.10) and $\varepsilon^{-1}(\nabla U_{\varepsilon}^{(1)} - \nabla U^{(1)})$ $\to \nabla U^{(2)}$ in $L_2(\mathbf{R}^d)^{d \times d}$ (see Remark 3.17). The integral term over the exterior domain vanishes due to the asymptotic behaviour of $U^{(1)}$. In order to compute $\partial_{\ell}^{(2)} \mathcal{L}(0, u_0, p_0)$, we use (5.11) to get

$$\frac{\mathcal{L}(\varepsilon, u_{0}, p_{\varepsilon}) - \mathcal{L}(0, u_{0}, p_{\varepsilon}) - \ell_{1}(\varepsilon)\partial_{\ell}^{(1)}\mathcal{L}(0, u_{0}, p_{0})}{\ell_{2}(\varepsilon)} =
\gamma_{f} \int_{\omega} \varepsilon^{-1}[(f_{1} \circ \Phi_{\varepsilon} - f_{2} \circ \Phi_{\varepsilon}) - (f_{1}(x_{0}) - f_{2}(x_{0}))] \cdot u_{0} \circ \Phi_{\varepsilon} dx
+ \gamma_{f} \int_{\omega} (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot \varepsilon^{-1}[u_{0} \circ \Phi_{\varepsilon} - u_{0}(x_{0})] dx
+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})\boldsymbol{\epsilon}(u_{0}) \circ \Phi_{\varepsilon} : \boldsymbol{\epsilon} \left(\varepsilon^{-1}\left[P_{\varepsilon}^{(1)} - P^{(1)}\right]\right) dx
+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})\varepsilon^{-1}[\boldsymbol{\epsilon}(u_{0}) \circ \Phi_{\varepsilon} - \boldsymbol{\epsilon}(u_{0})(x_{0})] : \boldsymbol{\epsilon}(P^{(1)}) dx
+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})\boldsymbol{\epsilon}(u_{0}) \circ \Phi_{\varepsilon} : \varepsilon^{-1}[\boldsymbol{\epsilon}(p_{0}) \circ \Phi_{\varepsilon} - \boldsymbol{\epsilon}(p_{0})(x_{0})] dx
+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})\varepsilon^{-1}[\boldsymbol{\epsilon}(u_{0}) \circ \Phi_{\varepsilon} - \boldsymbol{\epsilon}(u_{0})(x_{0})] : \boldsymbol{\epsilon}(p_{0})(x_{0}) dx
+ \int_{\omega} (f_{1} \circ \Phi_{\varepsilon} - f_{2} \circ \Phi_{\varepsilon}) \cdot \left(P_{\varepsilon}^{(1)}\right) dx
- \int_{\omega} (f_{1} \circ \Phi_{\varepsilon} - f_{2} \circ \Phi_{\varepsilon}) \cdot \varepsilon^{-1}[p_{0} \circ \Phi_{\varepsilon} - p_{0}(x_{0})] dx
- \int_{\omega} \varepsilon^{-1}[(f_{1} \circ \Phi_{\varepsilon} - f_{2} \circ \Phi_{\varepsilon}) - (f_{1}(x_{0}) - f_{2}(x_{0}))] \cdot p_{0}(x_{0}) dx.$$
(5.16)

Now, considering Theorem 4.4, item (2), we have $\varepsilon^{-1}[\epsilon(P_{\varepsilon}^{(1)}) - \epsilon(P^{(1)})] \rightarrow \epsilon(P^{(2)})$ in $L_2(\omega)^{d \times d}$ and by Theorem 4.2 and the Gagliardo–Nirenberg inequality, we get $P_{\varepsilon}^{(1)} \to P^{(1)}$ in $L_1(\omega)^d$. Thus, passing to the limit $\varepsilon \searrow 0$ in (5.16) we conclude

$$\partial_{\ell}^{(2)} \mathcal{L}(0, u_{0}, p_{0}) = \gamma_{f} \int_{\omega}^{\infty} \nabla[f_{1}(x_{0}) - f_{2}(x_{0})] x \cdot u_{0}(x_{0}) \, dx + \gamma_{f} \int_{\omega}^{\infty} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla u_{0}(x_{0}) x \, dx \\
+ \int_{\omega}^{\sigma} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : \epsilon(P^{(2)}) \, dx + \int_{\omega}^{\sigma} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla \epsilon(u_{0})(x_{0})x] : \epsilon(P^{(1)}) \, dx \\
+ \int_{\omega}^{\sigma} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : [\nabla (\epsilon(p_{0}))(x_{0})x] \, dx \\
+ \int_{\omega}^{\sigma} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla (\epsilon(u_{0}))(x_{0})x] : \epsilon(p_{0})(x_{0}) \, dx \\
- \int_{\omega}^{\sigma} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla p_{0}(x_{0}) x \, dx - \int_{\omega}^{\infty} \nabla [f_{1}(x_{0}) - f_{2}(x_{0})] x \cdot p_{0}(x_{0}) \, dx \\
- \int_{\omega}^{\sigma} (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot (P^{(1)}) \, dx.$$
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\text{Motion of } x = 0 \\
\text{Motion of$$

Thus, the second-order topological derivative is given by

$$d^{2}\mathcal{J}(\emptyset,\omega)(x_{0}) = \gamma_{f} \int_{\omega} \nabla[f_{1}(x_{0}) - f_{2}(x_{0})] x \cdot u_{0}(x_{0}) dx + \gamma_{f} \int_{\omega} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla u_{0}(x_{0}) x dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : \epsilon(P^{(2)}) dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla \epsilon(u_{0})(x_{0})x] : \epsilon(P^{(1)}) dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : [\nabla(\epsilon(p_{0}))(x_{0})x] dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla(\epsilon(u_{0}))(x_{0})x] : \epsilon(p_{0})(x_{0}) dx - \int_{\omega} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla p_{0}(x_{0})x dx - \int_{\omega} \nabla[f_{1}(x_{0}) - f_{2}(x_{0})] x \cdot p_{0}(x_{0}) dx - \int_{\omega} (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot (P^{(1)}) dx + 2\gamma_{g} \frac{1}{|\omega|} \int_{\mathbf{R}^{d}} \nabla U^{(1)} : \nabla U^{(2)} dx,$$
(5.18)

with $P^{(1)}$ defined in (4.5), $U^{(1)}$ defined in (3.42), $P^{(2)}$ defined in (4.14), (4.17) and $U^{(2)}$ defined in (3.66), (3.69).

5.2 Averaged adjoint method

We start with the first-order topological derivative. Therefore, let $\ell_1(\varepsilon) := |\omega_{\varepsilon}|$. By Proposition 2.4 item (1) we have

$$d\mathcal{J}(\emptyset,\omega)(x_0) = \mathcal{R}^{(1)}(u_0,q_0) + \partial_{\ell}^{(1)}\mathcal{L}(0,u_0,q_0),$$
(5.19)

where

$$\mathcal{R}^{(1)}(u_0, q_0) = \lim_{\epsilon \searrow 0} \frac{\mathcal{L}(\epsilon, u_0, q_\epsilon) - \mathcal{L}(\epsilon, u_0, q_0)}{\ell_1(\epsilon)},$$
$$\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, q_0) = \lim_{\epsilon \searrow 0} \frac{\mathcal{L}(\epsilon, u_0, q_0) - \mathcal{L}(0, u_0, q_0)}{\ell_1(\epsilon)},$$

if the above limits exist. Thus, we start computing $\mathcal{R}^{(1)}(u_0, q_0)$:

$$\frac{\mathcal{L}(\varepsilon, u_0, q_{\varepsilon}) - \mathcal{L}(\varepsilon, u_0, q_0)}{\ell_1(\varepsilon)} = \frac{1}{|\omega_{\varepsilon}|} [J_{\varepsilon}(u_0) + a_{\varepsilon}(u_0, q_{\varepsilon}) - f_{\varepsilon}(q_{\varepsilon}) - J_{\varepsilon}(u_0) - a_{\varepsilon}(u_0, q_0) + f_{\varepsilon}(q_0)]
= \frac{1}{|\omega_{\varepsilon}|} [a_{\varepsilon}(u_0, q_{\varepsilon} - q_0) - f_{\varepsilon}(q_{\varepsilon} - q_0)]
= \frac{1}{|\omega_{\varepsilon}|} \left[\int_{\omega_{\varepsilon}} (\mathbf{C}_1 - \mathbf{C}_2) \epsilon(u_0) : \epsilon(q_{\varepsilon} - q_0) \, dx - \int_{\omega_{\varepsilon}} (f_1 - f_2) \cdot (q_{\varepsilon} - q_0) \, dx \right]
= \int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \epsilon(u_0) \odot \Phi_{\varepsilon} : \epsilon\left(Q_{\varepsilon}^{(1)}\right) \, dx - \varepsilon \int_{\omega} (f_1 - f_2) \odot \Phi_{\varepsilon}\left(Q_{\varepsilon}^{(1)}\right) \, dx.$$
(5.20)

Since $u_0 \in C^3(B_{\delta}(x_0))$ for $\delta > 0$ small and by Theorem 4.6 $\epsilon(Q_{\epsilon}^{(1)}) \to \epsilon(Q^{(1)})$ in $L_2(\omega)^{d \times d}$ as ϵ tends to zero, we have

$$\lim_{\varepsilon \searrow 0} \int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0) \circ \boldsymbol{\Phi}_{\varepsilon} : \boldsymbol{\epsilon} \left(Q_{\varepsilon}^{(1)} \right) \, dx = \int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon} \left(Q^{(1)} \right) \, dx. \tag{5.21}$$

Furthermore, applying Hölder's inequality, Lemma 3.4 item (2), (3) and Theorem 4.6, one readily checks that $Q_{\varepsilon}^{(1)} \rightarrow Q^{(1)}$ in $L_1(\omega)^d$. Thus, we deduce

$$\lim_{\varepsilon \to 0} \varepsilon \int_{\omega} [(f_1 - f_2) \circ \Phi_{\varepsilon}] \cdot Q_{\varepsilon}^{(1)} \, dx = 0.$$
(5.22)

It follows that $\mathcal{R}^{(1)}(u_0, q_0) = \int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(Q^{(1)}) \, dx$. Next, we compute $\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, q_0)$. For this, we note for $\boldsymbol{\epsilon} > 0$:

Now, since u_0 , q_0 , f_1 , f_2 are smooth in a neighbourhood of x_0 , we get

$$\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, q_0) = \left[\gamma_f(f_1 - f_2) \cdot u_0 + (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0) : \boldsymbol{\epsilon}(q_0) - (f_1 - f_2) \cdot q_0 \right] (x_0).$$
(5.24)

Hence, the first-order topological derivative is given by

$$d\mathcal{J}(\emptyset,\omega)(x_0) = \oint_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(Q^{(1)}) dx + (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(q_0)(x_0) + \gamma_f (f_1(x_0) - f_2(x_0)) \cdot \boldsymbol{u}_0(x_0) - (f_1(x_0) - f_2(x_0)) \cdot q_0(x_0),$$
(5.25)

with $Q^{(1)}$ defined in (4.30), (4.33).

Remark 5.4. An elegant way to represent the topological derivative is by the use of a polarisation tensor (see Novotny and Sokolowski, 2013; Ammari *et al.*, 2005). For this, note that the mappings

$$\mathcal{F}^{1}: \mathbf{R}^{d \times d} \to \mathbf{R}^{d \times d}, \quad \zeta \mapsto \int_{\omega} \boldsymbol{\epsilon} \left(\widehat{Q}_{\zeta}^{(1)} \right) \, dx,$$
$$\mathcal{F}^{2}: \mathbf{R}^{d \times d} \to \mathbf{R}^{d \times d}, \quad \zeta \mapsto \int_{\omega} \boldsymbol{\epsilon} \left(\widetilde{Q}_{\zeta}^{(1)} \right) \, dx,$$

are linear, where $\widehat{Q}^{(1)}_{\zeta}$ solves

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(\widehat{Q}_{\zeta}^{(1)}) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \zeta \, dx \quad \text{for all } \boldsymbol{\varphi} \in \dot{BL}(\mathbf{R}^d)^d$$

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and $\tilde{Q}^{(1)}_{\boldsymbol{\zeta}}$ solves

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}\left(\tilde{Q}_{\zeta}^{(1)}\right) dx = -\gamma_g \int_{\mathbf{R}^d} \nabla U_{\zeta}^{(1)} : \nabla \boldsymbol{\varphi} \, dx \quad \text{for all } \boldsymbol{\varphi} \in \dot{BL}\left(\mathbf{R}^d\right)^d,$$

with $U^{(1)}_{\zeta}$ satisfying

$$\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon} \left(U_{\zeta}^{(1)} \right) : \boldsymbol{\epsilon}(\varphi) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \zeta : \boldsymbol{\epsilon}(\varphi) \, dx \quad \text{for all } \varphi \in \dot{BL} \left(\mathbf{R}^d \right)^d.$$
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Hence, there are tensors $\mathcal{P}^1, \mathcal{P}^2$ representing $\mathcal{F}^1, \mathcal{F}^2$ respectively, which we refer to as polarisation tensors. With their help we are able to rewrite (5.25) the following way:

$$d\mathcal{J}(\emptyset,\omega)(x_0) = (\mathbf{C}_1 - \mathbf{C}_2)\boldsymbol{\epsilon}(u_0)(x_0) : \mathcal{P}^1\boldsymbol{\epsilon}(q_0)(x_0) + (\mathbf{C}_1 - \mathbf{C}_2)\boldsymbol{\epsilon}(u_0)(x_0) : \mathcal{P}^2\boldsymbol{\epsilon}(u_0)(x_0)$$
(5.26)

+
$$[\gamma_f(f_1 - f_2) \cdot u_0 + (\mathbf{C}_1 - \mathbf{C}_2)\boldsymbol{\epsilon}(u_0) : \boldsymbol{\epsilon}(q_0) - (f_1 - f_2) \cdot q_0](x_0).$$
 (5.27)

Next we compute the second-order topological derivative. Therefore, let $\ell_2(\varepsilon) := \varepsilon \ell_1(\varepsilon)$. By Proposition 2.4 item (2) we have

$$d^{2}\mathcal{J}(\emptyset,\omega)(x_{0}) = \mathcal{R}^{(2)}(u_{0},q_{0}) + \partial_{\ell}^{(2)}\mathcal{L}(0,u_{0},q_{0}),$$
(5.28)

where

$$\mathcal{R}^{(2)}(u_0,q_0) = \lim_{\epsilon \searrow 0} \frac{\mathcal{L}(\epsilon, u_0, q_\epsilon) - \mathcal{L}(\epsilon, u_0, q_0) - \ell_1(\epsilon) \mathcal{R}^{(1)}(u_0, q_0)}{\ell_2(\epsilon)},$$

 $\partial_\ell^{(2)} \mathcal{L}(0, u_0, q_0) = \lim_{\epsilon \searrow 0} \frac{\mathcal{L}(\epsilon, u_0, q_0) - \mathcal{L}(0, u_0, q_0) - \ell_1(\epsilon) \partial_\ell^{(2)} \mathcal{L}(0, u_0, q_0)}{\ell_2(\epsilon)},$

if the above limits exist. We start computing $\mathcal{R}^{(2)}(u_0, q_0)$. Using (5.20) we get

$$\begin{aligned} \mathcal{R}^{(2)}(u_{0},q_{0}) &= \lim_{\epsilon \searrow 0} \left[\oint_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0}) \odot \Phi_{\varepsilon} : \epsilon \left(\varepsilon^{-1} Q_{\varepsilon}^{(1)} \right) dx - \int_{\omega} (f_{1} - f_{2}) \odot \Phi_{\varepsilon} \cdot \left(Q_{\varepsilon}^{(1)} \right) dx \\ &- \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : \epsilon \left(\varepsilon^{-1} Q^{(1)} \right) dx \right] \\ &= \lim_{\epsilon \searrow 0} \left[\int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \left[\varepsilon^{-1} (\epsilon(u_{0}) \odot \Phi_{\varepsilon} - \epsilon(u_{0})(x_{0})) \right] : \epsilon \left(Q_{\varepsilon}^{(1)} \right) dx \\ &+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : \epsilon \left(\varepsilon^{-1} Q_{\varepsilon}^{(1)} - \varepsilon^{-1} Q^{(1)} \right) dx \\ &+ \int_{\omega} (f_{1} - f_{2}) \odot \Phi_{\varepsilon} \cdot \left(Q_{\varepsilon}^{(1)} \right) dx \right] \\ &= \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla \epsilon(u_{0})(x_{0})x] : \epsilon (Q^{(1)}) dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : \epsilon (Q^{(2)}) dx \\ &- \int_{\omega} (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot (Q^{(1)}) dx, \end{aligned}$$
(5.29)

where we used $Q_{\varepsilon}^{(1)} \to Q^{(1)}$ in $L_1(\omega)^d$, $\epsilon(Q_{\varepsilon}^{(1)}) \to \epsilon(Q^{(1)})$ in $L_2(\omega)^d$ and by Theorem 4.8 $\epsilon^{-1}(\epsilon(Q_{\varepsilon}^{(1)}) - \epsilon(Q^{(1)})) \to \epsilon(Q^{(2)})$ in $L_2(\omega)^d$. Next, we compute $\partial_{\ell}^{(2)} \mathcal{L}(0, u_0, q_0)$:

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 \\
 \delta_{\ell}^{(2)} \mathcal{L}(0, u_{0}, q_{0}) = & \lim_{\epsilon \searrow 0} \left[\gamma_{f} \int_{\omega}^{\epsilon} \varepsilon^{-1} [(f_{1} - f_{2}) \circ \Phi_{\epsilon} \cdot u_{0} \circ \Phi_{\epsilon} - (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot u_{0}(x_{0})] \, dx \\
 + \int_{\omega}^{\epsilon} \varepsilon^{-1} [(\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0}) \circ \Phi_{\epsilon} : \epsilon(q_{0}) \circ \Phi_{\epsilon} - (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : \epsilon(q_{0})(x_{0})] \, dx \\
 - \int_{\omega}^{\epsilon} \varepsilon^{-1} [(f_{1} - f_{2}) \circ \Phi_{\epsilon} \cdot q_{0} \circ \Phi_{\epsilon} - (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot q_{0}(x_{0})] \, dx \\
 = & \gamma_{f} \int_{\omega}^{\epsilon} \nabla [(f_{1} - f_{2})](x_{0})x \cdot u_{0}(x_{0}) \, dx + \gamma_{f} \int_{\omega}^{\epsilon} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla u_{0}(x_{0})x \, dx \\
 + \int_{\omega}^{\epsilon} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla(\epsilon(u_{0}))(x_{0})x] : \epsilon(q_{0})(x_{0}) \, dx \\
 + \int_{\omega}^{\epsilon} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla(\epsilon(u_{0}))(x_{0})x] : k \\
 - \int_{\omega}^{\epsilon} [\nabla(f_{1} - f_{2})(x_{0})]x \cdot q_{0}(x_{0}) \, dx - \int_{\omega}^{\epsilon} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla q_{0}(x_{0})x \, dx, \\
 (5.30)
 \end{array}$$

where again we used the smoothness of u_0 , q_0 , f_1 , f_2 in a neighbourhood of x_0 in the last step. This is the claimed formula (5.23). Furthermore, combining (5.29) and (5.30), we obtain the final formula for the second-order topological derivative:

$$d^{2}\mathcal{J}(\emptyset, \omega)(x_{0}) = \gamma_{f} \int_{\omega} [\nabla(f_{1} - f_{2})(x_{0})]x \cdot u_{0}(x_{0}) dx + \gamma_{f} \int_{\omega} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla u_{0}(x_{0})x dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})[\nabla(\epsilon(u_{0}))(x_{0})x] : \epsilon(q_{0})(x_{0}) dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})\epsilon(u_{0})(x_{0}) : [\nabla(\epsilon(q_{0}))(x_{0})x] dx - \int_{\omega} [\nabla(f_{1} - f_{2})](x_{0})x \cdot q_{0}(x_{0}) dx - \int_{\omega} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla q_{0}(x_{0})x dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})[\nabla\epsilon(u_{0})(x_{0})x] : \epsilon(Q^{(1)}) dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2})\epsilon(u_{0})(x_{0}) : \epsilon(Q^{(2)}) dx - \int_{\omega} (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot (Q^{(1)}) dx,$$
(5.31)

with $Q^{(1)}$ defined in (4.30), (4.33) and $Q^{(2)}$ defined in (4.41), (4.44).

5.3 Delfour's method

At last, we consider Delfour's method to compute the topological derivative. Therefore, recall that by Proposition 2.7 item (1) we have

$$d\mathcal{J}(\emptyset,\omega)(x_0) = \mathcal{R}_1^{(1)}(u_0,p_0) + \mathcal{R}_2^{(1)}(u_0,p_0) + \partial_\ell^{(1)}\mathcal{L}(0,u_0,p_0),$$
(5.32)

where we let $\ell_1(\varepsilon) := |\omega_{\varepsilon}|$ and assume that the limits.

$$\mathcal{R}_{1}^{(1)}(u_{0},p_{0}) := \lim_{\varepsilon \searrow 0} \frac{1}{\ell_{1}(\varepsilon)} \int_{0}^{1} (\partial_{u}\mathcal{L}(\varepsilon,su_{\varepsilon}+(1-s)u_{0},p_{0}) - \partial_{u}\mathcal{L}(\varepsilon,u_{0},p_{0}))(u_{\varepsilon}-u_{0}) \, ds, \qquad (5.33)$$

$$\mathcal{R}_{2}^{(1)}(u_{0},p_{0}) := \lim_{\varepsilon \searrow 0} \frac{1}{\ell_{1}(\varepsilon)} (\partial_{u}\mathcal{L}(\varepsilon,u_{0},p_{0}) - \partial_{u}\mathcal{L}(0,u_{0},p_{0}))(u_{\varepsilon}-u_{0}), \tag{5.34}$$

$$\partial_{\ell}^{(1)}\mathcal{L}(0, u_0, p_0) := \lim_{\epsilon \searrow 0} \frac{1}{\ell_1(\epsilon)} (\mathcal{L}(\epsilon, u_0, p_0) - \mathcal{L}(0, u_0, p_0)), \tag{5.35} \qquad \begin{array}{c} \text{Adjoint-based} \\ \text{methods} \end{array}$$

exist. We now compute the limit of each term. Plugging in the definition of $\mathcal{L}(\varepsilon, u, v)$, we get for $\varepsilon > 0$,

$$\frac{1}{\ell_{1}(\varepsilon)} \int_{0}^{1} \left(\partial_{u} \mathcal{L}(\varepsilon, su_{\varepsilon} + (1-s)u_{0}, p_{0}) - \partial_{u} \mathcal{L}(\varepsilon, u_{0}, p_{0}) \right) (u_{\varepsilon} - u_{0}) \, ds \qquad 103$$

$$= \frac{1}{|\omega_{\varepsilon}|} \int_{0}^{1} \partial_{u} J(\varepsilon, su_{\varepsilon} + (1-s)u_{0}, p_{0}) (u_{\varepsilon} - u_{0}) - \partial_{u} J(\varepsilon, u_{0}, p_{0}) (u_{\varepsilon} - u_{0}) \, ds$$

$$= \frac{\varepsilon}{|\omega|} \gamma_{m} \|U_{\varepsilon}^{(1)}\|_{L_{2}(\Gamma_{\varepsilon}^{m})^{d}}^{2} + \frac{1}{|\omega|} \gamma_{g} \|\nabla U_{\varepsilon}^{(1)}\|_{L_{2}(\mathsf{D}_{\varepsilon})^{d \times d}}^{2}.$$
(5.36)

Hence, passing to the limit $\varepsilon \searrow 0$ yields $\mathcal{R}_1^{(1)}(u_0, p_0) = \frac{\gamma_g}{|\omega|} \|\nabla U^{(1)}\|_{L_2(\mathbf{R}^d)^{d \times d}}^2$ (see (5.9)). Furthermore, we have

$$\frac{1}{\ell_{1}(\varepsilon)}(\partial_{u}\mathcal{L}(\varepsilon,u_{0},p_{0})-\partial_{u}\mathcal{L}(0,u_{0},p_{0}))(u_{\varepsilon}-u_{0}) = \frac{1}{|\omega_{\varepsilon}|}\gamma_{f}\int_{\omega_{\varepsilon}}(f_{1}-f_{2})\cdot(u_{\varepsilon}-u_{0}) dx
+\frac{1}{|\omega_{\varepsilon}|}\int_{\omega_{\varepsilon}}(\mathbf{C}_{1}-\mathbf{C}_{2})\epsilon(u_{\varepsilon}-u_{0}):\epsilon(p_{0}) dx
= \epsilon\gamma_{f}\int_{\omega}(f_{1}\circ\Phi_{\varepsilon}-f_{2}\circ\Phi_{\varepsilon})\cdot\left(U_{\varepsilon}^{(1)}\right) dx
+\int_{\omega}(\mathbf{C}_{1}-\mathbf{C}_{2})\epsilon\left(U_{\varepsilon}^{(1)}\right):\epsilon(p_{0})\circ\Phi_{\varepsilon} dx.$$
(5.37)

Since $U_{\varepsilon}^{(1)} \to U^{(1)}$ in $L_1(\omega)^d$ and $\epsilon(U_{\varepsilon}^{(1)}) \to \epsilon(U^{(1)})$ in $L_2(\omega)^{d \times d}$ for $\varepsilon \searrow 0$, which can be seen similarly to the analogous results for $P^{(1)}$ and $Q^{(1)}$, it follows

$$\mathcal{R}_{2}^{(1)}(u_{0},p_{0}) = \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \boldsymbol{\epsilon} (U^{(1)}) : \boldsymbol{\epsilon}(p_{0})(x_{0}) \, dx.$$
(5.38)

A similar computation yields

$$\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0) = \left[\gamma_f(f_1 - f_2) \cdot u_0 + (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0) : \boldsymbol{\epsilon}(p_0) - (f_1 - f_2) \cdot p_0 \right](x_0).$$
(5.39)

A more detailed derivation of $\partial_{\ell}^{(1)} \mathcal{L}(0, u_0, p_0)$ can be found in (5.23) by substituting p_0 for q_0 . Combining these limits yields

$$d\mathcal{J}(\emptyset, \omega)(x_{0}) = -\int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(U^{(1)}) : \epsilon(p_{0})(x_{0}) dx + (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : \epsilon(p_{0})(x_{0}) + \gamma_{f}(f_{1}(x_{0}) - f_{2}(x_{0})) \cdot u_{0}(x_{0}) - (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot p_{0}(x_{0}) + \gamma_{g} \frac{1}{|\omega|} \int_{\mathbf{R}^{d}} |\nabla U^{(1)}|^{2} dx,$$
(5.40)

with $U^{(1)}$ defined in (3.42). Next, we compute the second-order topological derivative. In view of Proposition 2.7, item (2), we first show that the following limits exist:

$$\frac{\text{EC}}{39,1} \qquad \qquad \mathcal{R}_1^{(2)}(u_0, p_0) \coloneqq \lim_{\epsilon \searrow 0} \frac{1}{\ell_2(\epsilon)} \int_0^1 \partial_u \mathcal{L}(\epsilon, su_\epsilon + (1-s)u_0, p_0) \tag{5.41}$$

$$-\partial_u \mathcal{L}(\varepsilon, u_0, p_0)(u_{\varepsilon} - u_0) ds - \ell_1(\varepsilon) \mathcal{R}_1^{(1)}(u_0, p_0),$$

$$\mathcal{R}_{2}^{(2)}(u_{0},p_{0}) := \lim_{\varepsilon \searrow 0} \frac{1}{\ell_{2}(\varepsilon)} \Big[(\partial_{u}\mathcal{L}(\varepsilon,u_{0},p_{0}) - \partial_{u}\mathcal{L}(0,u_{0},p_{0}))(u_{\varepsilon}-u_{0}) - \ell_{1}(\varepsilon)\mathcal{R}_{2}^{(1)}(u_{0},p_{0}) \Big], \quad (5.42)$$

$$\partial_{\ell}^{(2)}\mathcal{L}(0,u_0,p_0) := \lim_{\varepsilon \searrow 0} \frac{1}{\ell_2(\varepsilon)} \left[\mathcal{L}(\varepsilon,u_0,p_0) - \mathcal{L}(0,u_0,p_0) - \ell_1(\varepsilon)\partial_{\ell}^{(1)}\mathcal{L}(0,u_0,p_0) \right], \quad (5.43)$$

where $\ell_2(\varepsilon) := \varepsilon \ell_1(\varepsilon)$. Then the topological derivative is given by

$$d^{2}\mathcal{J}(\Omega)(x_{0}) = \mathcal{R}_{1}^{(2)}(u_{0}, p_{0}) + \mathcal{R}_{2}^{(2)}(u_{0}, p_{0}) + \partial_{\ell}^{(2)}\mathcal{L}(0, u_{0}, p_{0})$$

Similar to (5.15) it follows that

$$\mathcal{R}_1^{(2)}(u_0, p_0) = 2\gamma_g \frac{1}{|\omega|} \int_{\mathbf{R}^d} \nabla U^{(1)} : \nabla U^{(2)} \, dx$$

Furthermore, we have

$$\frac{1}{\ell_{2}(\varepsilon)} (\partial_{u} \mathcal{L}(\varepsilon, u_{0}, p_{0}) - \partial_{u} \mathcal{L}(0, u_{0}, p_{0})) \quad (u_{\varepsilon} - u_{0}) - \ell_{1}(\varepsilon) \mathcal{R}_{2}^{(1)}(u_{0}, p_{0})$$

$$= \gamma_{f} \int_{\omega} (f_{1} \circ \Phi_{\varepsilon} - f_{2} \circ \Phi_{\varepsilon}) \cdot \left(U_{\varepsilon}^{(1)}\right) dx$$

$$+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon \left(\varepsilon^{-1} \left[U_{\varepsilon}^{(1)} - U^{(1)}\right]\right) : \epsilon(p_{0}) \circ \Phi_{\varepsilon} dx$$

$$+ \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon \left(U^{(1)}\right) : \left[\varepsilon^{-1}(\epsilon(p_{0}) \circ \Phi_{\varepsilon} - \epsilon(p_{0})(x_{0}))\right] dx.$$
(5.44)

Hence, passing to the limit $\varepsilon \searrow 0$, we deduce

$$\mathcal{R}_{2}^{(2)}(u_{0},p_{0}) = \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \boldsymbol{\epsilon} (U^{(2)}) : \boldsymbol{\epsilon}(p_{0})(x_{0}) \, dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \boldsymbol{\epsilon} (U^{(1)})$$

$$: [\nabla \boldsymbol{\epsilon}(p_{0})(x_{0})x] \, dx + \gamma_{f} - \int_{\omega} (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot U^{(1)} \, dx, \qquad (5.45)$$

where we used $\varepsilon^{-1}[\epsilon(U_{\varepsilon}^{(1)}) - \epsilon(U^{(1)})] \rightarrow \epsilon(U^{(2)})$ in $L_2(\omega)^{d \times d}$ and $U_{\varepsilon}^{(1)} \rightarrow U^{(1)}$ in $L_1(\omega)^d$. Additionally, from (5.30) we get

$$\partial_{\ell}^{(2)} \mathcal{L}(0, u_{0}, p_{0}) = \gamma_{f} \int_{\omega} \nabla [f_{1}(x_{0}) - f_{2}(x_{0})] x \cdot u_{0}(x_{0}) \, dx + \gamma_{f} \int_{\omega} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla u_{0}(x_{0}) x \, dx \\ + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla (\boldsymbol{\epsilon}(u_{0}))(x_{0})x] : \boldsymbol{\epsilon}(p_{0})(x_{0}) \, dx \\ + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \boldsymbol{\epsilon}(u_{0})(x_{0}) : [\nabla (\boldsymbol{\epsilon}(p_{0}))(x_{0})x] \, dx \\ - \int_{\omega} \nabla [f_{1}(x_{0}) - f_{2}(x_{0})] x \cdot p_{0}(x_{0}) \, dx - \int_{\omega} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla p_{0}(x_{0}) x \, dx.$$
(5.46)

We obtain

$$d^{2}\mathcal{J}(\emptyset,\omega)(x_{0}) = \gamma_{f} \int_{\omega} (f_{1}(x_{0}) - f_{2}(x_{0})) \cdot U^{(1)} dx + 2\gamma_{g} \frac{1}{|\omega|} \int_{\mathbf{R}^{d}} \nabla U^{(1)} : \nabla U^{(2)} dx \qquad \text{methods} \\ + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(U^{(2)}) : \epsilon(p_{0})(x_{0}) dx + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(U^{(1)}) : [\nabla\epsilon(p_{0})(x_{0})x] dx \\ + \gamma_{f} \int_{\omega} \nabla [f_{1}(x_{0}) - f_{2}(x_{0})]x \cdot u_{0}(x_{0}) dx + \gamma_{f} \int_{\omega} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla u_{0}(x_{0})x dx \qquad 105 \\ + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) [\nabla(\epsilon(u_{0}))(x_{0})x] : \epsilon(p_{0})(x_{0}) dx \\ + \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(u_{0})(x_{0}) : [\nabla(\epsilon(p_{0}))(x_{0})x] dx \\ - \int_{\omega} \nabla [f_{1}(x_{0}) - f_{2}(x_{0})]x \cdot p_{0}(x_{0}) dx - \int_{\omega} [f_{1}(x_{0}) - f_{2}(x_{0})] \cdot \nabla p_{0}(x_{0})x dx, \qquad (5.47)$$

Adjoint-based

with $U^{(1)}$ defined in (3.42) and $U^{(2)}$ defined in (3.66), (3.69). This finishes the proof of the computation of the second-order topological derivative using Delfour's method.

Remark 5.5. We would like to point out that using the defining equations of the boundary layer correctors, one can show that all three expressions of the second-order topological derivative coincide and therefore all methods lead to the same result. To get an idea, we show that the first-order topological derivative of Amstutz' approach and the averaged adjoint method are the same. Plugging in $\varphi = Q^{(1)}$ in (3.42) yields

$$\int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(u_0)(x_0) : \boldsymbol{\epsilon}(Q^{(1)}) \ dx = -\int_{\mathbf{R}^d} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(U^{(1)}) : \boldsymbol{\epsilon}(Q^{(1)}) \ dx.$$

Additionally, by choosing $\varphi = P^{(1)}$ in(4.5) and $\varphi = U^{(1)}$ in (4.30), (4.33) we get

$$\int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \boldsymbol{\epsilon}(u_{0})(x_{0}) : \boldsymbol{\epsilon}(P^{(1)}) dx + \int_{\mathbf{R}^{d}} |\nabla U^{(1)}|^{2} dx$$

$$= \underbrace{-\int_{\mathbf{R}^{d}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(U^{(1)}) : \boldsymbol{\epsilon}(P^{(1)}) dx + \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) \boldsymbol{\epsilon}(q_{0})(x_{0}) : \boldsymbol{\epsilon}(U^{(1)}) dx}_{=0}$$

$$- \int_{\mathbf{R}^{d}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(U^{(1)}) : \boldsymbol{\epsilon}(Q^{(1)}) dx.$$

Now using $p_0 = q_0$ it follows that both results (5.13), (5.25) coincide.

6. Conclusion

In the present work we review three different methods to compute the second-order topological derivative and illustrate their methodologies by applying them to a linear elasticity model. To give a better insight into the differences of these methods, the cost functional consists of three terms: the compliance, a L_2 tracking type over a part of the

Neumann boundary and a gradient tracking type over the whole domain, whereas the first one is linear and the latter two are quadratic.

Amstutz' method to compute the topological derivative requires besides the analysis of the direct state u_{ε} also the analysis of the adjoint state p_{ε} . Even though this seems to lead to additional work, we would like to point out that, due to the ε -dependence of the defining equation of the adjoint state variable, the analysis of p_{ε} resembles the analysis of the direct state and can be done in a similar way. The computation of the topological derivative for the compliance term is straightforward, whereas checking the occurring limits for the nonlinearities requires the asymptotic analysis of u_{ε} on the whole domain.

The averaged adjoint method shifts the work from the computation of the topological derivative to the asymptotic analysis of the averaged adjoint variable q_{ε} . Since the defining equation depends on the state variable u_{ε} , the asymptotic analysis of p_{ε} does not resemble the analysis of u_{ε} and therefore needs to be treated differently. In fact, we would like to mention that again the non-linearities of the cost functional are the reason for additional work during this process. When it comes to the computation of the topological derivative, the averaged adjoint method simplifies the procedure as it only requires convergence of q_{ε} on a small subdomain of size ε .

Finally, Delfour's method resembles Amstutz' method as it requires the asymptotic analysis of u_{ε} on the whole domain, yet it does not need the analysis of the adjoint state p_{ε} . This advantage seems to come with the shortcoming, that this method is only applicable to a selective set of cost functions.

To recapitulate, each method proposed in this work has some advantages and disadvantages over the others. The decision on which method fits the actual problem setting the best greatly depends on the actual cost function as well as the properties of the underlying partial differential equation.

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Appendix

Here we derive equations satisfied by the variations of the adjoint and average adjoint variable respectively.

A1 Derivation and estimation of Equation (4.10)

In order to compute G_e^1 , we subtract (4.3) and (4.4) to obtain

$$\int_{\mathsf{D}} \mathbf{C}_{\omega_{\varepsilon}} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(p_{\varepsilon} - p_0) \, dx = \int_{\omega_{\varepsilon}} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(p_0) \, dx + \gamma_f \int_{\omega_{\varepsilon}} (f_2 - f_1) \cdot \boldsymbol{\varphi} \, dx,$$
(A.1)

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$. Next we change variables according to the transformation $y = \Phi_{\varepsilon}(x)$, multiply with ε^{1-d} and subtract

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon}(P^{(1)}) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon}(p_0)(x_0) \, dx + \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_2^\top \boldsymbol{\epsilon}(P^{(1)}) n \cdot \varphi \, dS \quad (A.2)$$

to conclude

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon} \left(P_{\varepsilon}^{(1)} - P^{(1)} \right) \, dx = G_{\varepsilon}^{1}(\boldsymbol{\varphi}), \tag{A.3}$$

for all $\varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d$ with the notation

$$G_{\varepsilon}^{1}(\varphi) = \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) \boldsymbol{\epsilon}(\varphi) : [\boldsymbol{\epsilon}(p_{0}) \circ \boldsymbol{\Phi}_{\varepsilon} - \boldsymbol{\epsilon}(p_{0})(x_{0})] dx \qquad \qquad \text{Adjoint-based} \\ + \boldsymbol{\epsilon} \gamma_{f} \int_{\omega} (f_{2} - f_{1}) \circ \boldsymbol{\Phi}_{\varepsilon} \cdot \varphi \, dx \qquad \qquad (A.4)$$

$$-\int_{\Gamma_{N,e}} \mathbf{C}_2^{ op} \, \boldsymbol{\epsilon} \left(P^{(1)}
ight) n \cdot \boldsymbol{\varphi} \; dS.$$

Now we can find a constant C > 0, such that the following estimates hold:

- (1) $\left| \int_{\infty} (\mathbf{C}_2 \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : [\boldsymbol{\epsilon}(\boldsymbol{p}_0) \circ \boldsymbol{\Phi}_{\boldsymbol{\varepsilon}} \boldsymbol{\epsilon}(\boldsymbol{p}_0)(\boldsymbol{x}_0)] d\boldsymbol{x} \right| \le C \boldsymbol{\varepsilon} \|\boldsymbol{\varphi}\|_{\boldsymbol{\varepsilon}}$, which follows from a Taylor's expansion of $\epsilon(p_0) \circ \Phi \varepsilon$ in x_0 and Hölder's inequality.
- (2) $|\varepsilon \gamma_f \int_{\omega} (f_2 f_1) \circ \Phi_{\varepsilon} \cdot \varphi \, dx| \le C \varepsilon ||\varphi||_{\varepsilon}$ for d = 3 and $|\varepsilon \gamma_f \int_{\omega} (f_2 f_1) \circ \Phi_{\varepsilon} \cdot \varphi \, dx| \le C \varepsilon ||\varphi||_{\varepsilon}^{1-\alpha}$, for d = 2 which is a consequence of Hölder's inequality and Lemma 3.4 item (2) and (3).(3) $\left| \int_{\Gamma_{N,e}} \mathbf{C}_{2}^{\top} \epsilon(P^{(1)}) n \cdot \varphi \, dS \right| \le C \varepsilon^{\frac{d}{2}} \|\varphi\|_{e^{*}} \text{ which follows from Hölder's inequality, Lemma 3.4 item (4)}$
- and Lemma 3.5, item (3) with m = d 1.

Combining the previous estimates yields

$$\|G_{\varepsilon}^{1}\| \le \begin{cases} C\varepsilon & \text{for } d = 3, \\ C\varepsilon^{1-\alpha} & \text{for } d = 2. \end{cases}$$
(A.5)

A2 Derivation and estimation of Equation (4.23)

We start by dividing (Section A3) by ε and subtract (4.13), (4.20), which can be formulated on the domain D_{e} by a change of variables. Next we subtract (4.14) (4.17), whereas these equations can be restricted to the domain D_{e} by splitting the integral over \mathbf{R}^{d} and integrating by parts in the exterior domain. These operations leave us with

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon} \left(\varepsilon P_{\varepsilon}^{(3)} \right) dx = G_{\varepsilon}^{2}(\boldsymbol{\varphi}) + G_{\varepsilon}^{3}(\boldsymbol{\varphi}), \tag{A.6}$$

for all $\varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d$ where

$$G_{\varepsilon}^{2}(\varphi) = \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) \boldsymbol{\epsilon}(\varphi) : [\varepsilon^{-1}(\boldsymbol{\epsilon}(p_{0}) \circ \Phi_{\varepsilon} - \boldsymbol{\epsilon}(p_{0})(x_{0})) - \nabla \varepsilon(p_{0})(x_{0})x] dx$$

$$+ \gamma_{f} \int_{\omega} [(f_{2} - f_{1}) \circ \Phi_{\varepsilon} - (f_{2}(x_{0}) - f_{1}(x_{0}))] \cdot \varphi dx \qquad (A.7)$$

$$+ \varepsilon^{d-1} \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) \boldsymbol{\epsilon}(\varphi) : [\boldsymbol{\epsilon}(p^{(1)}) \circ \Phi_{\varepsilon} + \boldsymbol{\epsilon}(p^{(2)}) \circ \Phi_{\varepsilon}] dx,$$

$$G_{\varepsilon}^{3}(\varphi) = -\varepsilon^{-1} \int_{\Gamma_{N,\varepsilon}} [\mathbf{C}_{2}^{\top} \boldsymbol{\epsilon}(P^{(1)}) - \varepsilon^{d} \mathbf{C}_{2}^{\top} \boldsymbol{\epsilon}(S^{(1)})(\varepsilon x)] n \cdot \varphi dS$$

$$- \int_{\Gamma_{N,\varepsilon}} [\mathbf{C}_{2}^{\top} \boldsymbol{\epsilon}(P^{(2)}) - \varepsilon^{d-1} \mathbf{C}_{2}^{\top} \boldsymbol{\epsilon}(S^{(2)})(\varepsilon x)] n \cdot \varphi dS. \qquad (A.8)$$

Now we want to estimate the norm of G_{e}^k $k \in \{2, 3\}$. Therefore let $\varphi \in H^1_{\Gamma_e}(\mathsf{D}_{e})^d$.

(1) Since p_0 is three times differentiable in a neighbourhood of x_0 , there is a constant C > 0, such that $|\varepsilon^{-1}(\epsilon(p_0) \circ \Phi_{\varepsilon} - \epsilon(p_0)(x_0)) - \nabla \epsilon(p_0)(x_0)x| \le C\varepsilon$, for $x \in \omega$. Hence, Hölder's inequality yields

$$\left| \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \left[\boldsymbol{\varepsilon}^{-1}(\boldsymbol{\epsilon}(p_0) \bigcirc \boldsymbol{\Phi}_{\boldsymbol{\varepsilon}} - \boldsymbol{\epsilon}(p_0)(x_0)) - \nabla \boldsymbol{\epsilon}(p_0)(x_0) x \right] \, dx \right| \le C \boldsymbol{\varepsilon} \|\boldsymbol{\varphi}\|_{\boldsymbol{\varepsilon}}.$$
(A.9)

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(2) A Taylor expansion of $(f_2 - f_1) \circ \Phi_{\varepsilon}$ at x_0 , Hölder's inequality and Lemma 3.4 item (2) yield

$$\left|\gamma_{f} \int_{\omega} \left[(f_{2} - f_{1}) \bigcirc \Phi_{\varepsilon} - (f_{2}(x_{0}) - f_{1}(x_{0})) \right] \cdot \varphi \, dx \right| \leq C \varepsilon \|\varphi\|_{\varepsilon}, \tag{A.10}$$

for a constant C > 0.

(3) Furthermore, by Hölder's inequality we get

$$\left|\varepsilon^{d-1} \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \left[\boldsymbol{\epsilon}(\boldsymbol{p}^{(1)}) \bigcirc \boldsymbol{\Phi}_{\varepsilon} + \boldsymbol{\epsilon}(\boldsymbol{p}^{(2)}) \bigcirc \boldsymbol{\Phi}_{\varepsilon}\right] dx \right| \leq C \varepsilon \|\boldsymbol{\varphi}\|_{\varepsilon}, \tag{A.11}$$

for a constant C > 0.

Combining the above results leaves us with $||G_{\varepsilon}^2|| \leq C\varepsilon$ for a constant C > 0. Next we consider the boundary integral terms:

(4) From Hölder's inequality, Lemma 3.5 item (3) with m = d and the scaled trace inequality we get

$$\left| \varepsilon^{-1} \int_{\Gamma_{N,\varepsilon}} \left[\mathbf{C}_{2}^{\top} \, \boldsymbol{\epsilon} \left(P^{(1)} \right) - \varepsilon^{d} \mathbf{C}_{2}^{\top} \, \boldsymbol{\epsilon} \left(S^{(1)} \right) (\varepsilon x) \right] n \cdot \varphi \, dS \right| \leq C \varepsilon^{\frac{d}{2}} \|\varphi\|_{\varepsilon}, \tag{A.12}$$

for a constant C > 0.

(5) Similarly, we deduce from Lemma 3.5 item (3) with m = d - 1 that there is a constant C > 0, such that

$$\left| \int_{\Gamma_{N\varepsilon}} \left[\mathbf{C}_{2}^{\top} \boldsymbol{\epsilon} \left(P^{(2)} \right) - \boldsymbol{\varepsilon}^{d-1} \mathbf{C}_{2}^{\top} \boldsymbol{\epsilon} \left(S^{(2)} \right) (\boldsymbol{\varepsilon} \boldsymbol{x}) \right] \boldsymbol{n} \cdot \boldsymbol{\varphi} \, dS \right| \leq C \boldsymbol{\varepsilon}^{\frac{d}{2}} \| \boldsymbol{\varphi} \|_{\boldsymbol{\varepsilon}}. \tag{A.13}$$

Thus, these estimates result in $||G_{\varepsilon}^3|| \leq C\varepsilon$ for a constant C > 0.

A3 Derivation and estimation of Equation (4.37) In order to compute a governing equation for $Q_{\varepsilon}^{(1)} - Q^{(1)}$, we start by subtracting (4.28) and (4.29). Rearranging these terms leaves us with

$$\int_{D} \mathbf{C}_{\omega_{\varepsilon}} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(q_{\varepsilon} - q_{0}) \, dx = \int_{\omega_{\varepsilon}} (\mathbf{C}_{2} - \mathbf{C}_{1}) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(q_{0}) \, dx \\ + \gamma_{f} \int_{\omega_{\varepsilon}} (f_{2} - f_{1}) \cdot \boldsymbol{\varphi} \, dx \\ - \gamma_{m} \int_{\Gamma_{m}} (u_{\varepsilon} - u_{0}) \cdot \boldsymbol{\varphi} \, dS \\ - \gamma_{g} \int_{D} [\nabla u_{\varepsilon} - \nabla u_{0}] : \nabla \boldsymbol{\varphi} \, dx,$$
(A.14)

for all $\varphi \in H^1_{\Gamma}(\mathsf{D})^d$. Thus, considering the definition of $U^{(1)}_{\varepsilon}$, a change of variables followed by subtracting

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(Q^{(1)}) \, dx = \int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(q_0)(x_0) \, dx - \gamma_g \int_{\mathsf{D}_{\varepsilon}} \nabla U^{(1)} : \nabla \boldsymbol{\varphi} \, dx \\ + \int_{\Gamma_{N_{\varepsilon}}} \mathbf{C}_2^{\mathsf{T}} \, \boldsymbol{\epsilon}(Q^{(1)}) n \cdot \boldsymbol{\varphi} \, dS + \int_{\Gamma_{N_{\varepsilon}}} \nabla U^{(1)} n \cdot \boldsymbol{\varphi} \, dS \\ + \int_{\mathbf{R}^d \setminus \mathsf{D}_{\varepsilon}} \underbrace{\left[\operatorname{div}(\mathbf{C}_2^{\mathsf{T}} \, \boldsymbol{\epsilon}(Q^{(1)})) + \gamma_g \Delta U^{(1)} \right]}_{=0} \cdot \boldsymbol{\varphi} \, dx,$$
(A.15)

vields

$$\int_{D_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}\left(\boldsymbol{\varepsilon}Q_{\varepsilon}^{(2)}\right) dx = G_{\varepsilon}^{4}(\boldsymbol{\varphi}), \qquad (A.16) \qquad \text{Adjoint-based} \\ \text{methods} \\ G_{\varepsilon}^{4}(\boldsymbol{\varphi}) = \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1})\boldsymbol{\epsilon}(\boldsymbol{\varphi}) : [\boldsymbol{\epsilon}(q_{0}) \circ \boldsymbol{\Phi}_{\varepsilon} - \boldsymbol{\epsilon}(q_{0})(x_{0})] dx \\ + \boldsymbol{\epsilon} \boldsymbol{\gamma}_{f} \int_{\omega} (f_{2} \circ \boldsymbol{\Phi}_{\varepsilon} - f_{1} \circ \boldsymbol{\Phi}_{\varepsilon}) \cdot \boldsymbol{\varphi} dx \qquad 111 \\ - \boldsymbol{\epsilon} \boldsymbol{\gamma}_{m} \int_{\Gamma_{m,\varepsilon}} \left(U_{\varepsilon}^{(1)}\right) \cdot \boldsymbol{\varphi} dS \\ - \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2}^{\mathsf{T}} \boldsymbol{\epsilon}(Q^{(1)}) \boldsymbol{n} \cdot \boldsymbol{\varphi} dS \\ - \gamma_{g} \int_{\Gamma_{N,\varepsilon}} \nabla U^{(1)} \boldsymbol{n} \cdot \boldsymbol{\varphi} dS \\ - \gamma_{g} \int_{D_{\varepsilon}} \left(\nabla U_{\varepsilon}^{(1)} - \nabla U^{(1)}\right) : \nabla \boldsymbol{\varphi} dx, \qquad (A.17)$$

.

where

for all
$$\varphi \in H^1_{\Gamma_{\epsilon}}(\mathsf{D}_{\epsilon})^d$$
.

Now let $\varphi \in H^1_{\Gamma_{\varepsilon}}(D_{\varepsilon})^d$. There is a constant C > 0 independent of ε and φ , such that.

- (1) $\left|\int_{\omega} (\mathbf{C}_2 \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : [\boldsymbol{\epsilon}(q_0) \circ \boldsymbol{\Phi}_{\varepsilon} \boldsymbol{\epsilon}(q_0)(x_0)] dx\right| \le C \varepsilon \|\boldsymbol{\varphi}\|_{\varepsilon}$, which can be seen by a Taylor's expansion of q^0 in x^0 and Hölder's inequality.
- (2) |εγ_f∫_ω(f₂ Φ_ε − f₁ Φ_ε) · φ dx| ≤ Cε ||φ||_ε, which is a consequence of Hölder's inequality and Lemma 3.4 item (2).
- (3) $|\int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2}^{\top} \epsilon(Q^{(1)}) n \cdot \varphi \, dS| \le C \varepsilon^{\frac{1}{2}} \|\varphi\|_{\varepsilon}$, which is a consequence of Hölder's inequality, Lemma 3.5 item (3) with m = d 2 and the scaled trace inequality.
- (4) $|\gamma_{e} \int_{\Gamma_{v}} \nabla U^{(1)} n \cdot \varphi \, dS| \leq C \epsilon^{\frac{d}{2}} \|\varphi\|_{e}$, which can be seen similarly.
- (5) $|\varepsilon \gamma_m \int_{\Gamma_{m,\varepsilon}} (U_{\varepsilon}^{(1)}) \cdot \varphi \, dS| \leq C \varepsilon \|\varphi\|_{\varepsilon}$, which follows from Hölder's inequality, splitting $\|U_{\varepsilon}^{(1)}\|_{L_2(\Gamma_{m,\varepsilon})^d} \leq \|U_{\varepsilon}^{(1)} U^{(1)}\|_{L_2(\Gamma_{m,\varepsilon})^d} + \|U^{(1)}\|_{L_2(\Gamma_{m,\varepsilon})^d}$, the scaled trace inequality, Theorem 3.10 and Lemma 3.5 item (1) with m = d 1.
- (6) $|\gamma_g \int_{D_{\varepsilon}} (\nabla U_{\varepsilon}^{(1)} \nabla U^{(1)}) : \nabla \varphi \, dx| \le C \varepsilon ||\varphi||_{\varepsilon}$, which is a consequence of Hölder's inequality and Theorem 3.10.

Combining the above results leaves us with

$$\|G_{\varepsilon}^4\|_{\cdot} \leq C\varepsilon^{\frac{1}{2}}$$

A4 Derivation and estimation of Equation (4.51)

Due to the high number of terms, we derive the governing equation in more detail. Therefore, we formulate (4.40), (4.47), (4.48), (4.41) and (4.44) on the domain D_e by scaling arguments and splitting of the integral domain respectively, to get

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon} \left(\varepsilon^{d-3} q^{(1)} \circ \Phi_{\varepsilon} \right) dx = -\varepsilon^{d-2} \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2}^{\top} \boldsymbol{\epsilon} \left(T^{(1)} \right) (\varepsilon x) n \cdot \varphi \, dS + \varepsilon^{d-2} \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon} \left(q^{(1)} \right) \circ \Phi_{\varepsilon} \, dx,$$
(A.18)

$$\frac{\text{EC}}{39,1} \qquad \qquad \int_{D_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}\left(\widehat{\boldsymbol{Q}}^{(2)}\right) d\boldsymbol{x} = \quad \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : [\nabla \boldsymbol{\epsilon}(q_{0})(\boldsymbol{x}_{0})\boldsymbol{x}] d\boldsymbol{x} \\ - \gamma_{g} \int_{D_{\varepsilon}} \nabla U^{(2)} : \nabla \boldsymbol{\varphi} \, dS \\ + \gamma_{g} \int_{\Gamma_{N,\varepsilon}} \nabla U^{(2)} \boldsymbol{n} \cdot \boldsymbol{\varphi} \, dS \\ + \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2}^{\top} \, \boldsymbol{\epsilon}(\widehat{\boldsymbol{Q}}^{(2)}) \boldsymbol{n} \cdot \boldsymbol{\varphi} \, dS,$$
(A.19)

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}\left(\tilde{\boldsymbol{Q}}^{(2)}\right) d\boldsymbol{x} = \gamma_{f} \int_{\omega} [f_{2}(\boldsymbol{x}_{0}) - f_{1}(\boldsymbol{x}_{0})] \cdot \boldsymbol{\varphi} d\boldsymbol{x} + \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2}^{\top} \boldsymbol{\epsilon}\left(\tilde{\boldsymbol{Q}}^{(2)}\right) \boldsymbol{n} \cdot \boldsymbol{\varphi} d\boldsymbol{S},$$
(A.20)

$$\begin{split} \int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \quad \boldsymbol{\epsilon} \left(\varepsilon^{d-2} q^{(2)} \circ \mathbf{\Phi}_{\varepsilon} \right) dx &= -\varepsilon^{d-1} \gamma_{m} \int_{\Gamma_{m,\varepsilon}} R^{(1)}(\varepsilon x) \cdot \boldsymbol{\varphi} \, dS - \varepsilon \gamma_{m} \int_{\Gamma_{m,\varepsilon}} \left(\varepsilon^{d-2} u^{(1)} \circ \mathbf{\Phi}_{\varepsilon} \right) \cdot \boldsymbol{\varphi} \, dS \\ &- \varepsilon^{d-1} \gamma_{m} \int_{\Gamma_{m,\varepsilon}} R^{(2)}(\varepsilon x) \cdot \boldsymbol{\varphi} \, dS - \varepsilon \gamma_{m} \int_{\Gamma_{m,\varepsilon}} \left(\varepsilon^{d-2} u^{(2)} \circ \mathbf{\Phi}_{\varepsilon} \right) \cdot \boldsymbol{\varphi} \, dS \\ &- \varepsilon^{d-2} \gamma_{g} \int_{\mathsf{D}_{\varepsilon}} \nabla \left(u^{(1)} \circ \mathbf{\Phi}_{\varepsilon} \right) : \nabla \boldsymbol{\varphi} \, dx - \varepsilon^{d-2} \gamma_{g} \int_{\mathsf{D}_{\varepsilon}} \nabla \left(u^{(2)} \circ \mathbf{\Phi}_{\varepsilon} \right) : \nabla \boldsymbol{\varphi} \, dx \\ &- \varepsilon^{d-1} \gamma_{g} \int_{\Gamma_{N,\varepsilon}} \nabla \left(R^{(1)} \right) (\varepsilon x) n \cdot \boldsymbol{\varphi} \, dS - \varepsilon^{d-1} \gamma_{g} \int_{\Gamma_{N,\varepsilon}} \nabla \left(R^{(2)} \right) (\varepsilon x) n \cdot \boldsymbol{\varphi} \, dS \\ &+ \varepsilon^{d-1} \int_{\omega} \left(\mathbf{C}_{1} - \mathbf{C}_{2} \right) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}\left(q^{(2)} \right) \circ \mathbf{\Phi}_{\varepsilon} \, dx. \end{split}$$

$$(A.21)$$

Now dividing (A.16), (A.17) by ε and subtracting (A.18)–(A.21) leaves us with

$$\int_{\mathsf{D}_{\varepsilon}} \mathbf{C}_{\omega} \boldsymbol{\epsilon}(\varphi) : \boldsymbol{\epsilon}(V_{\varepsilon}) \, dx = G_{\varepsilon}^{5}(\varphi) + G_{\varepsilon}^{6}(\varphi), \tag{A.22}$$

where we remember the simplified notation $V_{\varepsilon} := \varepsilon^{-1}[Q_{\varepsilon}^{(1)} - Q^{(1)}] - \varepsilon^{d-3}q^{(1)} \circ \Phi_{\varepsilon} - Q^{(2)} - \varepsilon^{d-2}q^{(2)} \circ \Phi_{\varepsilon}$ and

$$\begin{aligned} G_{\varepsilon}^{5}(\varphi) &= \int_{\omega} (\mathbf{C}_{2} - \mathbf{C}_{1}) \epsilon(\varphi) : \left[\varepsilon^{-1}(\epsilon(q_{0}) \circ \Phi_{\varepsilon} - \epsilon(q_{0})(x_{0})) - \nabla \varepsilon(q_{0})(x_{0})x \right] dx \\ &+ \gamma_{f} \int_{\omega} \left[(f_{2} \circ \Phi_{\varepsilon} - f_{1} \circ \Phi_{\varepsilon}) - (f_{2}(x_{0}) - f_{1}(x_{0})) \right] \cdot \varphi \, dx \\ &- \gamma_{g} \int_{D_{\varepsilon}} \left[\varepsilon^{-1} \left(\nabla U_{\varepsilon}^{(1)} - \nabla U^{(1)} \right) - \nabla \left(\varepsilon^{d-2} u^{(1)} \circ \Phi_{\varepsilon} \right) - \nabla U^{(2)} - \nabla \left(\varepsilon^{d-2} u^{(2)} \circ \Phi_{\varepsilon} \right) \right] : \nabla \varphi \, dx \\ &+ \varepsilon^{d-2} \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(\varphi) : \epsilon(q^{(1)}) \circ \Phi_{\varepsilon} \, dx \\ &+ \varepsilon^{d-1} \int_{\omega} (\mathbf{C}_{1} - \mathbf{C}_{2}) \epsilon(\varphi) : \epsilon(q^{(2)}) \circ \Phi_{\varepsilon} \, dx, \end{aligned}$$
(A.23)

$$\begin{aligned}
G_{\varepsilon}^{6}(\varphi) &= -\varepsilon \gamma_{m} \int_{\Gamma_{m,\varepsilon}} \left(\varepsilon^{-1} U_{\varepsilon}^{(1)} - \varepsilon^{d-2} R^{(1)}(\varepsilon x) - \varepsilon^{d-2} u^{(1)} \circ T_{\varepsilon} - \varepsilon^{d-2} R^{(2)}(\varepsilon x) - \varepsilon^{d-2} u^{(2)} \circ T_{\varepsilon} \right) \cdot \varphi \, dS & \text{Adjoint-based} \\
&= \varepsilon^{-1} \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2}^{\top} \left[\epsilon(Q^{(1)}) - \varepsilon^{d-1} \epsilon(T^{(1)})(\varepsilon x) \right] n \cdot \varphi \, dS & -\int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2}^{\top} \epsilon(Q^{(2)}) n \cdot \varphi \, dS & \text{I13} \\
&= -\gamma_{g} \varepsilon^{-1} \int_{\Gamma_{N,\varepsilon}} [\nabla U^{(1)} - \varepsilon^{d} \nabla (R^{(1)})(\varepsilon x)] n \cdot \varphi \, dS & \text{I13} \\
&= -\gamma_{g} \int_{\Gamma_{N,\varepsilon}} [\nabla U^{(2)} - \varepsilon^{d-1} \nabla (R^{(2)})(\varepsilon x)] n \cdot \varphi \, dS. & \text{(A.24)}
\end{aligned}$$

In the following let $\varphi \in H^1_{\Gamma_{\varepsilon}}(\mathsf{D}_{\varepsilon})^d$ and *C* denote a sufficiently large constant independent of φ and ε . We now want to estimate the operator norm of $G^k_{\varepsilon}, k \in \{5, 6\}$ with respect to $\|\cdot\|_{\varepsilon}$:

(1) A Taylor's expansion and Hölder's inequality yield

$$\left|\int_{\omega} (\mathbf{C}_2 - \mathbf{C}_1) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \left[\boldsymbol{\varepsilon}^{-1}(\boldsymbol{\epsilon}(q_0) \circ \boldsymbol{\Phi}_{\varepsilon} - \boldsymbol{\epsilon}(q_0)(x_0)) - \nabla \boldsymbol{\varepsilon}(q_0)(x_0) \boldsymbol{x} \right] d\boldsymbol{x} \right| \leq C \boldsymbol{\varepsilon} \|\boldsymbol{\varphi}\|_{\varepsilon}.$$

(2) A Taylor's expansion followed by an application of Hölder's inequality with respect to $p = 2^*$ and Lemma 3.4 item (2) yield

$$\left|\gamma_f \int_{\omega} \left[(f_2 \circ \Phi_{\varepsilon} - f_1 \circ \Phi_{\varepsilon}) - (f_2(x_0) - f_1(x_0)) \right] \cdot \varphi \, dx \right| \leq C \varepsilon \|\varphi\|_{\varepsilon}.$$

(3) From Theorem 3.16 we deduce

$$\left|\gamma_{g}\int_{\mathsf{D}_{\varepsilon}}\left[\varepsilon^{-1}\left(\nabla U_{\varepsilon}^{(1)}-\nabla U^{(1)}\right)-\nabla\left(\varepsilon^{d-2}u^{(1)}\circ\Phi_{\varepsilon}\right)-\nabla U^{(2)}-\nabla\left(\varepsilon^{d-2}u^{(2)}\circ\Phi_{\varepsilon}\right)\right]:\nabla\varphi\,dx\right|\leq C\varepsilon\|\varphi\|_{\varepsilon}.$$

(4) Furthermore, from Hölder's inequality it follows

$$\left|\varepsilon^{d-2}\int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(q^{(1)}) \circ \boldsymbol{\Phi}_{\varepsilon} \, dx\right| \leq C \varepsilon \|\boldsymbol{\varphi}\|_{\varepsilon}.$$

(5) Similarly, one gets

$$\left|\varepsilon^{d-1}\int_{\omega} (\mathbf{C}_1 - \mathbf{C}_2) \boldsymbol{\epsilon}(\boldsymbol{\varphi}) : \boldsymbol{\epsilon}(q^{(2)}) \circ \Phi_{\varepsilon} dx\right| \leq C \varepsilon \|\boldsymbol{\varphi}\|_{\varepsilon}.$$

Combining these estimates, we get $\|G_{\varepsilon}^{5}\| \leq C\varepsilon$. Next we consider the boundary integral terms.

(6) By smuggling in $\varepsilon^{-1}U^{(1)}$ and $U^{(2)}$ we get

$$\begin{split} & \left| \epsilon \gamma_m \int_{\Gamma_{m,\varepsilon}} \left(\epsilon^{-1} U_{\varepsilon}^{(1)} - \epsilon^{d-2} R^{(1)}(\epsilon x) - \epsilon^{d-2} u^{(1)} \circ \Phi_{\varepsilon} - \epsilon^{d-2} R^{(2)}(\epsilon x) - \epsilon^{d-2} u^{(2)} \circ \Phi_{\varepsilon} \right) \cdot \varphi \; dS \right| \leq \\ & \left| \epsilon \gamma_m \int_{\Gamma_{m,\varepsilon}} \left(\epsilon^{-1} U_{\varepsilon}^{(1)} - \epsilon^{-1} U^{(1)} - \epsilon^{d-2} u^{(1)} \circ \Phi_{\varepsilon} - U^{(2)} - \epsilon^{d-2} u^{(2)} \circ \Phi_{\varepsilon} \right) \cdot \varphi \; dS \right| \\ & + \left| \epsilon \gamma_m \int_{\Gamma_{m,\varepsilon}} \left(\epsilon^{-1} U^{(1)} - \epsilon^{d-2} R^{(1)}(\epsilon x) \right) \cdot \varphi \; dS \right| \\ & + \left| \epsilon \gamma_m \int_{\Gamma_{m,\varepsilon}} (U^{(2)} - \epsilon^{d-2} R^{(2)}(\epsilon x)) \cdot \varphi \; dS \right|. \end{split}$$

The first term on the right-hand side can be estimated by Hölder's inequality, the scaled trace inequality and Theorem 3.16, whereas the remaining terms can be estimated by Hölder's inequality, the scaled trace inequality and Lemma 3.5 item (1). Thus we conclude

$$\varepsilon \gamma_m \int_{\Gamma_{m,\varepsilon}} \left(\varepsilon^{-1} U_{\varepsilon}^{(1)} - \varepsilon^{d-2} R^{(1)}(\varepsilon x) - \varepsilon^{d-2} u^{(1)} \circ \Phi_{\varepsilon} - \varepsilon^{d-2} R^{(2)}(\varepsilon x) - \varepsilon^{d-2} u^{(2)} \circ \Phi_{\varepsilon} \right) \cdot \varphi \, dS \bigg| \leq C \varepsilon \|\varphi\|_{\varepsilon}.$$

ī.

(7) A similar computation to Lemma 3.5 and the scaled trace inequality yield

$$\left| \varepsilon^{-1} \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_{2}^{\top} \left[\boldsymbol{\epsilon} \left(Q^{(1)} \right) - \varepsilon^{d-1} \boldsymbol{\epsilon} \left(T^{(1)} \right) (\varepsilon x) \right] n \cdot \boldsymbol{\varphi} \, dS \right| \leq C \varepsilon^{\frac{1}{2}} \ln \left(\varepsilon^{-1} \right) \| \boldsymbol{\varphi} \|_{\varepsilon}.$$

(8) A similar argument shows

$$\left| \int_{\Gamma_{N,\varepsilon}} \mathbf{C}_2^\top \, \boldsymbol{\epsilon} \big(Q^{(2)} \big) n \cdot \varphi \, dS \right| \leq C \varepsilon^{\frac{1}{2}} \ln \big(\varepsilon^{-1} \big) \| \varphi \|_{\varepsilon}.$$

(9) Furthermore, the remaining terms can be estimated by Hölder's inequality, the scaled trace inequality and Lemma 3.5 item (3) with m = d - 1 and m = d respectively, to deduce

$$\left| \gamma_{g} \varepsilon^{-1} \int_{\Gamma_{N,\varepsilon}} \left[\nabla U^{(1)} - \varepsilon^{d} \nabla \left(R^{(1)} \right) (\varepsilon x) \right] n \cdot \varphi \, dS \right| \leq C \varepsilon^{\frac{d}{2}} \|\varphi\|_{\varepsilon},$$
$$\left| \gamma_{g} \int_{\Gamma_{N,\varepsilon}} \left[\nabla U^{(2)} - \varepsilon^{d-1} \nabla \left(R^{(2)} \right) (\varepsilon x) \right] n \cdot \varphi \, dS \right| \leq C \varepsilon^{\frac{d}{2}} \|\varphi\|_{\varepsilon}.$$

Hence, we conclude $||G_{\varepsilon}^{6}|| \leq C\varepsilon^{\frac{1}{2}}\ln(\varepsilon^{-1}).$

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