The Second-Order Eulerian Derivative of a Shape Functional of a Free Boundary Problem

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***Abstract*—The Kohn-Vogelius objective functional that evolves from the exterior Bernoulli free boundary problem is being studied. The first-order Eulerian derivative of this functional is being recalled. Assuming the sufficient regularity of domains and functions, this paper computes the shape derivatives of all functions involved, and derives the second-order Eulerian derivative of the functional by using the approach of Sokolowski and Zolesio. We also use a domain differentiation technique as an alternative way to validate our result. It is shown that the second-order Eulerian derivative satisfies a structure theorem. As a supplement, the explicit form of the derivative is also derived.**

***Index Terms*—Bernoulli problem, boundary value problems, perturbation of identity, shape derivative, material derivative, Eulerian derivative.**

I. Introduction

In this paper, we are interested in two-dimensional exterior Bernoulli free boundary problems. These problems arise in various applications such as electrochemical machining, fluid mechanics, optimal insulation, electrical impedance tomography, among others [8], [10], [15], [18], [19], [35]. The exterior Bernoulli problem is formulated as follows: Given a negative constant λ and a bounded connected domain $A \subset \mathbb{R}^2$ having a fixed boundary $\Gamma := \partial A$, we wish to find (i) a bounded connected domain $B \subset \mathbb{R}^2$ with a free boundary Σ such that $\bar{A} \subset B$, and (ii) a function $u : \Omega \to \mathbb{R}$, where $\Omega = B \backslash \bar{A}$, satisfying the following conditions:

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega, \\ u = 1 & \text{on } \Gamma, \\ u = 0 & \text{on } \Sigma, \\ \dfrac{\partial u}{\partial \mathbf{n}} = \lambda & \text{on } \Sigma. \end{cases} \tag{1}$$

Here, $\mathbf{n}$ refers to the outward unit normal vector to Σ. Details about the exterior Bernoulli problems can be seen, for instance, in [1], [2], [7], [9], [18], [20], [21], [24], [33].

The presence of overdetermined conditions on Σ makes the problem difficult to solve. Shape optimization method, however, is an established tool in solving such problems, and one way to reformulate the problem is as follows:

$$\min_{\Omega} J(\Omega) \equiv \min_{\Omega} \frac{1}{2} \int_{\Omega} |\nabla(u_D - u_N)|^2 \, \mathrm{d}x \tag{2}$$

over all admissible domains Ω, where the state function u_D is the solution to the Dirichlet problem:

$$\begin{cases} -\Delta u_D = 0 & \text{in } \Omega, \\ u_D = 1 & \text{on } \Gamma, \\ u_D = 0 & \text{on } \Sigma, \end{cases} \tag{3}$$

and the state function u_N is the solution to the Neumann problem:

$$\begin{cases} -\Delta u_N = 0 & \text{in } \Omega, \\ u_N = 1 & \text{on } \Gamma, \\ \dfrac{\partial u_N}{\partial \mathbf{n}} = \lambda & \text{on } \Sigma. \end{cases} \tag{4}$$

The functional J is commonly known as *Kohn-Vogelius cost functional* because Kohn and Vogelius were among the first to use it in the context of inverse conductivity problems [27], as mentioned by Eppler and Harbrecht in their paper [16].

Minimizing a shape functional requires, most of the time, some gradient information and Hessian. For the functional under consideration, the first-order Eulerian derivative had already been carried out (cf. [4]). This was done through variational means similar to the techniques developed in [20], [21], [25], wherein the Hölder continuity of the state variables satisfying the Dirichlet and Neumann problems are considered; however, we did not introduce any adjoint variables in our work. The Eulerian derivative was also computed using material or shape derivatives of the states (cf. [1], [5]).

In 2012, Kasumba and Kunisch [26] used the techniques in [25] to compute the second-order Eulerian derivative of a particular shape functional without using the shape derivative of the state variable. In their approach, Hölder continuity of the given state variable and the corresponding adjoint variable were used. However, this strategy of Kasumba and Kunisch seems to be difficult to apply in computing the second-order Eulerian derivative of the Kohn-Vogelius functional. The difficulty arises from the complexity of the first-order Eulerian derivative and the presence of two boundary value problems. So we used instead the approach of Sokolowski and Zolesio [32] wherein material derivatives, as well as shape derivatives of the state variables, are highly involved. The material and shape derivatives of the unit normal vector $\mathbf{n}$, the unit tangent vector τ and the mean curvature κ of Σ were also computed and applied in the derivation of the second-order derivative. The explicit form of the second-order derivative for general domains was finally obtained using Steklov-Poincare operators. To further validate our result, we also used a different technique which uses a domain differentiation formula. Contrary however to Simon [31] and Eppler [14] we managed not to use the second

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variations of the states in characterizing the second-order Eulerian derivative of J. Interestingly, the computed second-order Eulerian derivative has symmetric and nonsymmetric terms – a structure that was given in [11] and further investigated by Novruzi and Pierre [29]. Other techniques in computing the second-order Eulerian derivative of J in the direction of normal deformation fields to Σ are seen in the papers [5], [6] and [17].

II. TOOLS FROM SHAPE CALCULUS

In this work we consider two-dimensional bounded connected domains Ω of class $C^{k,1}$, $k \geq 1$, and these domains are subsets of a hold-all domain U. Moreover, Ω is an annulus having a fixed boundary Γ which is disjoint from another boundary Σ, which is freely moving. We also consider deformation fields $\mathbf{V}$ belonging to the space Θ defined by

$$\Theta = \left\{ \mathbf{V} \in C^{1,1}(\bar{U}, \mathbb{R}^2) : \mathbf{V}|_{\Gamma \cup \partial U} = 0 \right\}. \tag{5}$$

We deform Ω via the perturbation of identity operator

$$T_t : \bar{U} \to \mathbb{R}^2, \qquad T_t(x) = x + t\mathbf{V}(x), x \in \bar{U} \tag{6}$$

where $\mathbf{V} \in \Theta$. For $t = 0$, we have the reference domain $\Omega := \Omega_0$, with a fixed boundary $\Gamma := \Gamma_0$ and a free boundary $\Sigma := \Sigma_0$. For a given $t > 0$ we denote the deformed domain to be Ω_t, with a fixed boundary Γ_t and a free boundary Σ_t.

Throughout the paper, the following notations are used:

$$\left\{ \begin{array}{lcl} I_t(x) & = & \det DT_t(x), \ x \in \bar{U}, \\ M_t(x) & = & (DT_t(x))^{-T}, \ x \in \bar{U}, \\ A_t(x) & = & I_t M_t^T M_t(x), \ x \in \bar{U}, \\ w_t(x) & = & I_t(x)|(DT_t(x))^{-T}\mathbf{n}(x)|, \ x \in \Sigma \end{array} \right. \tag{7}$$

The determinant I_t of the transformation T_t has the following property.

Lemma 2.1 (see [20], [25]): Consider the operator T_t defined by (6), where $\mathbf{V} \in \Theta$, which is described by (5). Then

i. $I_t = 1 + t \operatorname{div} \mathbf{V} + t^2 \det D\mathbf{V}$, and
ii. there exists $t_V, \alpha_1, \alpha_2 > 0$ such that $0 < \alpha_1 \leq I_t(x) \leq \alpha_2$, for $|t| \leq t_V, x \in U$.

Using Lemma 2.1 one can show the following:

Theorem 2.2 (see [4]): Let Ω and U be nonempty bounded open connected subsets of $\mathbb{R}^2$ with Lipschitz continuous boundaries, such that $\bar{\Omega} \subseteq U$, and $\partial\Omega$ is the union of two disjoint boundaries Γ and Σ. Let T_t be defined as in (6) where $\mathbf{V}$ belongs to Θ, defined by (5).

Then for sufficiently small t,

1) $T_t : \bar{U} \to \bar{U}$ is a homeomorphism,
2) $T_t : U \to U$ is a $C^{1,1}$ diffeomorphism, and in particular, $T_t : \Omega \to \Omega_t$ is a $C^{1,1}$ diffeomorphism,
3) $\Gamma_t = T_t(\Gamma) = \Gamma$, and
4) $\partial\Omega_t = \Gamma \cup T_t(\Sigma)$.

Remark 2.3: We note the following observations for fixed, sufficiently small t: $I_t \in C^{0,1}(\bar{U})$; $M_t, M_t^T \in C(\bar{U}; \mathbb{R}^{2\times 2})$; $A_t \in C(\bar{U}; \mathbb{R}^{2\times 2})$; and $w_t \in C(\Sigma; \mathbb{R})$.
Here are some useful properties of T_t.

Lemma 2.4 (see [20], [25]): Consider the transformation T_t, where the fixed vector field $\mathbf{V}$ belongs to Θ, defined in (5). Then the exists $t_V > 0$ such that T_t and the functions in (7) restricted to the interval $I_V = (-t_V, t_V)$ have the following regularity and properties:

(1.) $t \mapsto T_t \in C^1(I_V, C^{1,1}(\bar{U}, \mathbb{R}^2))$.
(2.) $t \mapsto I_t \in C^1(I_V, C^{0,1}(\bar{U}))$.
(3.) $t \mapsto T_t^{-1} \in C(I_V, C^1(\bar{U}, \mathbb{R}^2))$.
(4.) $t \mapsto w_t \in C^1(I_V, C(\Sigma))$.
(5.) $t \mapsto A_t \in C(I_V, C(\bar{U}, \mathbb{R}^{2\times 2}))$.
(6.) There is $\beta > 0$ such that $A_t(x) \geq \beta I$ for $x \in U$.
(7.) $\frac{d}{dt} T_t|_{t=0} = \mathbf{V}$.
(8.) $\frac{d}{dt} T_t^{-1}|_{t=0} = -\mathbf{V}$.
(9.) $\frac{d}{dt} DT_t|_{t=0} = D\mathbf{V}$.
(10.) $\frac{d}{dt} (DT_t)^{-1}|_{t=0} = -D\mathbf{V}$.
(11.) $\frac{d}{dt} I_t|_{t=0} = \operatorname{div} \mathbf{V}$.
(12.) $\frac{d}{dt} A_t|_{t=0} = A$, where $A = (\operatorname{div} \mathbf{V})I - (D\mathbf{V} + (D\mathbf{V})^T$
(13.) $\lim_{t\to 0} w_t = 1$.
(14.) $\frac{d}{dt} w_t|_{t=0} = \operatorname{div}_\Sigma \mathbf{V}$
where $\operatorname{div}_\Sigma \mathbf{V} = \operatorname{div} \mathbf{V}|_\Sigma - (D\mathbf{V}\mathbf{n}) \cdot \mathbf{n}$.

In the discussion of the second-order Eulerian derivative we need to perturb the reference domain twice. Hence we consider the transformations $T_t^{\mathbf{V}} : \bar{U} \to \mathbb{R}^2$ and $T_s^{\mathbf{W}} : \bar{U} \to \mathbb{R}^2$ defined by $T_t^{\mathbf{V}}(x) = (I + t\mathbf{V})(x)$, and $T_s^{\mathbf{W}}(y) = (I + s\mathbf{W})(y), x, y \in \bar{U}$, respectively where $\mathbf{V}, \mathbf{W} \in \Theta$. For the sake of simplicity, unless stated otherwise, we denote T_t the transformation $T_t^{\mathbf{V}}$ in the direction $\mathbf{V}$. Also, we let $T_s := T_s^{\mathbf{W}}$. Using Theorem 2.2, the mapping $T_{t,s} := T_t \circ T_s : \Omega \to \Omega_{t,s}$, defined by

$$\begin{array}{rcl} T_{t,s}(x) & := & T_t(T_s(x)) \\ & = & x + s\mathbf{W}(x) + t\mathbf{V}(x + s\mathbf{W}(x)), \ x \in \Omega, \end{array} \tag{8}$$

may be proven to be a $C^{1,1}$ diffeomorphism. We define the perturbed domain $\Omega_{t,s}$ as:

$$\Omega_{t,s} := T_t(T_s(\Omega)) := \{T_{t,s}(x) : x \in \Omega\}.$$

Hence, for sufficiently small t and s, $\Omega_t, \Omega_{t,s}$ are of class $C^{1,1}$, and they are contained in U.

A. The Method of Mapping

If u is defined in Ω and u_t is defined in Ω_t then the direct comparison of u_t with u is generally not possible since the functions are defined on different domains. To overcome this difficulty one maps u_t back to Ω by composing it with T_t; that is, one defines $u_t \circ T_t : \Omega \to \mathbb{R}$. With this new mapping one can define the material and the shape derivatives of states, the domain and boundary integral transformations, derivatives of integrals, as well as the Eulerian derivatives of the shape functional.

1) Material and shape derivatives: The material and shape derivatives of state variables are defined as follows [22], [34]:

Definition 2.5: Let u be defined in $[0, t_V] \times U$. An element $\dot{u} \in H^k(\Omega)$, called the *material derivative* of u, is defined as

$$\begin{aligned}\dot{u}(x) &:= \dot{u}(0,x) := \lim_{t\to 0^+}\frac{u(t,T_t(x))-u(0,x)}{t}\\ &= \frac{d}{dt}u(t,x+t\mathbf{V}(x))\bigg|_{t=0}\end{aligned}$$

if the limit exists in $(H^k(\Omega))$.

Remark 2.6: The material derivative can be written as

$$\dot{u}(x)=\lim_{t\to 0^+}\frac{u_t\circ T_t(x)-u(x)}{t}=\frac{d}{dt}(u_t\circ T_t(x))\bigg|_{t=0}. \quad (9)$$

It characterizes the behavior of the function u at $x\in\Omega\subset U$ in the direction $\mathbf{V}(x)$. Generally, for bounded C^k-domains, if $u(x):=u(0,x)\in W^{m,p}(U)$, $m\in[0,k]$, $1\le p<\infty$ then $u\circ T_t\in W^{m,p}(\Omega)$ and if the limit (9) exists in $W^{m,p}(\Omega)$ then $\dot{u}(x)\in W^{m,p}(\Omega)$.

Definition 2.7: Let u be defined in $[0,t_V]\times U$. An element $u'\in H^k(\Omega)$ is called the *shape derivative* of u at Ω in the direction $\mathbf{V}$, if the following limit exists in $H^k(\Omega)$:

$$u'(x):=u'(0,x):=\lim_{t\to 0^+}\frac{u(t,x)-u(0,x)}{t}. \quad (10)$$

Remark 2.8: The shape derivative of u is also defined as follows:

$$u'(x):=\frac{\partial}{\partial t}u_t(x)\bigg|_{t=0}.$$

We note that if $\dot{u}$ and $\nabla u\cdot V$ exist in $H^k(\Omega)$ then the shape derivative can be written as

$$u'(x)=\dot{u}(x)-(\nabla u\cdot\mathbf{V})(x). \quad (11)$$

In general, if $\dot{u}(x)$ and $\nabla u\cdot\mathbf{V}(x)$ both exist in $W^{m,p}(\Omega)$, then $u'(x)$ also exists in that space.

Remark 2.9: The Definitions of material and shape derivative of real-valued functions can be extended to vector-valued functions. Analogous to Definition 2.5, assuming that $\mathbf{u}:[0,t_V]\times U\to\mathbb{R}^n$ belongs to $H^k(\Omega;\mathbb{R}^n)$ then its material derivative in the direction $\mathbf{V}$ can be written as

$$\begin{aligned}\dot{\mathbf{u}}(x) &:= \dot{\mathbf{u}}(\Omega;\mathbf{V}) = \lim_{t\to 0^+}\frac{\mathbf{u}(t,T_t(x))-\mathbf{u}(0,x)}{t}\\ &= \frac{d}{dt}\mathbf{u}(t,x+t\mathbf{V}(x))\bigg|_{t=0} \quad (12)\end{aligned}$$

if the limit exists in $(H^k(\Omega,\mathbb{R}^n))$. If its shape derivative also exists then one can have the following relation:

$$\mathbf{u}'(x)=\dot{\mathbf{u}}(x)-(D\mathbf{u}\mathbf{V})(x). \quad (13)$$

If $\mathbf{u}=(u_1,u_2)$ then its norm is given by $|\mathbf{u}|_{H^k(\Omega,\mathbb{R}^2)}=|u_1|_{H^k(\Omega)}+|u_2|_{H^k(\Omega)}$ for $k\ge 0$.

2) Domain and boundary transformations:

Lemma 2.10 (see [25], [32]):

1. Let $\varphi_t\in L^1(\Omega_t)$. Then $\varphi_t\circ T_t\in L^1(\Omega)$ and

$$\int_{\Omega_t}\varphi_t\,\mathrm{d}x_t=\int_\Omega\varphi_t\circ T_t I_t\,\mathrm{d}x.$$

2. Let $\varphi_t\in L^1(\partial\Omega_t)$. Then $\varphi_t\circ T_t\in L^1(\partial\Omega)$ and

$$\int_{\partial\Omega_t}\varphi_t\,\mathrm{d}s_t=\int_{\partial\Omega}\varphi_t\circ T_t w_t\,\mathrm{d}s,$$

where I_t and w_t are defined in (7).

Some tangential Calculus: Here are some properties of tangential differential operators which are used in this work (cf. [11], [23], [32]). Let Γ be a boundary of a bounded domain $\Omega\subset\mathbb{R}^n$.

Definition 2.11: The *tangential gradient* of $f\in C^1(\Gamma)$ is given by

$$\nabla_\Gamma f:=\nabla F|_\Gamma-\frac{\partial F}{\partial\mathbf{n}}\mathbf{n}\in C(\Gamma,\mathbb{R}^n), \quad (14)$$

where F is any C^1 the extension of f into a neighborhood of Γ.

Definition 2.12: The *tangential Jacobian matrix* of a vector function $\mathbf{v}\in C^1(\Gamma,\mathbb{R}^n)$ is given by

$$D_\Gamma\mathbf{v}=D\mathbf{V}|_\Gamma-(D\mathbf{V}\mathbf{n})\mathbf{n}^T\in C(\Gamma,\mathbb{R}^{n\times n}), \quad (15)$$

where $\mathbf{V}$ is any C^1 the extension of $\mathbf{v}$ into a neighborhood of Γ.

Definition 2.13: For a vector function $\mathbf{v}\in C^1(\Gamma,\mathbb{R}^n)$, its *tangential divergence* on Γ is given by

$$\operatorname{div}_\Gamma\mathbf{v}=\operatorname{div}\mathbf{V}|_\Gamma-D\mathbf{V}\mathbf{n}\cdot\mathbf{n}\ \in C(\Gamma), \quad (16)$$

where $\mathbf{V}$ is any C^1 the extension of $\mathbf{v}$ into a neighborhood of Γ.

Remark 2.14: The details of the existence of the extension F and $\mathbf{V}$ can be found in [11, pp.361 - 366]. We note that the above Definitions do not depend on the choice of the extension.

Lemma 2.15 (see [32]): Consider a C^2 domain Ω with boundary $\Gamma:=\partial\Omega$. Then for $u\in H^1(\Gamma)$ and $\mathbf{V}\in C^1(\Gamma,\mathbb{R}^n)$ the following identities hold:

$$(1)\quad \operatorname{div}_\Gamma(u\mathbf{V})=\nabla_\Gamma u\cdot\mathbf{V}+u\operatorname{div}_\Gamma\mathbf{V} \quad (17)$$

$$(2)\quad \int_\Gamma\operatorname{div}_\Gamma\mathbf{V}\,\mathrm{d}s=\int_\Gamma\kappa\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s \quad (18)$$

$$(3)\quad \int_\Gamma(u\operatorname{div}_\Gamma\mathbf{V}+\nabla_\Gamma u\cdot\mathbf{V})\,\mathrm{d}s=\int_\Gamma\kappa u\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s \quad (19)$$

$$(4)\quad \int_\Gamma\nabla_\Gamma u\cdot\mathbf{V}\,\mathrm{d}s=-\int_\Gamma u\operatorname{div}_\Gamma\mathbf{V}\,\mathrm{d}s,\ \text{where } \mathbf{V}\cdot\mathbf{n}=0 \quad (20)$$

Remark 2.16: In Lemma 2.15, the first identity is called *tangential divergence formula*, the second is commonly known as *tangential Stoke's formula*, and the third is referred to as *tangential Green's formula*. These formulas are also valid for $C^{1,1}$ domains.

3) Domain Differentiation Formula: The Theorem below is valid for $C^{0,1}$ domains. For proof, see [32].

Theorem 2.17: Let $u\in C(I_V,W^{1,1}(U))$ and suppose $\dot{u}(0,\cdot):=\frac{d}{dt}u(t,T_t(\cdot))\big|_{t=0}$ exists in $L^1(U)$. Then

$$\begin{aligned}\frac{d}{dt}\int_{\Omega_t}u(t,x)\,\mathrm{d}x\bigg|_{t=0} &= \int_\Omega u'(0,x)\,\mathrm{d}x\\ &\quad+\int_\Sigma u(0,s)\mathbf{V}\cdot\mathbf{n}\,\mathrm{d}s. \quad (21)\end{aligned}$$

4) The Eulerian derivatives: The Eulerian derivatives of a shape functional are defined as follows (cf. [11], [20], [34]):

Definition 2.18: The *first-order Eulerian derivative* of a shape functional $J:\Omega\to\mathbb{R}$ at the domain Ω in the direction of the deformation field $\mathbf{V}$ is given by

$$dJ(\Omega;\mathbf{V}):=\lim_{t\to 0^+}\frac{J(\Omega_t)-J(\Omega)}{t}, \quad (22)$$

if the limit exists.

The *second-order Eulerian derivative* of J at the domain Ω in the direction of the deformation fields $\mathbf{V}$ and $\mathbf{W}$ is given by

$$d^2J(\Omega;\mathbf{V},\mathbf{W}) = \lim_{s\to 0^+} \frac{dJ(\Omega_s(\mathbf{W}),\mathbf{V}) - dJ(\Omega;\mathbf{V})}{s} \quad (23)$$

if the limit exists.

Remark 2.19: J is said to be shape differentiable at Ω if $dJ(\Omega;\mathbf{V})$ exists for all $\mathbf{V}$ and is linear and continuous with respect to $\mathbf{V}$. It is twice shape differentiable if for all $\mathbf{V}$ and $\mathbf{W}$, $d^2J(\Omega;\mathbf{V},\mathbf{W})$ exists and if $d^2J(\Omega;\mathbf{V},\mathbf{W})$ is bilinear and continuous with respect to $\mathbf{V}$ and $\mathbf{W}$.

B. Structure of the second-order Eulerian derivative

In [11, p.384], it was shown by using the perturbation of identity that the expression $d^2J(\Omega;\mathbf{V},\mathbf{W})$ can be decomposed into a symmetric term plus a nonsymmetric part. The nonsymmetric part is determined by gradient applied to the deformation field $D\mathbf{V}\mathbf{W}$. This is further investigated by Novruzi and Pierre [29]. Their approach is based on the perturbation of identity technique presented in [28], [30]. The structure of the shape derivative of functional J uses the fact that any regular small perturbation $\Omega_\theta := (I+\theta)(\Omega)$ of a smooth domain Ω (where θ is sufficiently smooth mapping from $\mathbb{R}^n$ to $\mathbb{R}^n$) can be uniquely represented up to a "shift" on Γ by a normal deformation to Γ.

For any $l \in \mathbb{N}, 1 \le l \le k$, we denote

$$G^{k-l}(\Gamma,\Gamma) = \left\{ g \in C^{k-l}(\Gamma,\mathbb{R}^n) : g(\Gamma) \subset \Gamma \right\}. \quad (24)$$

Lemma 2.20: Let Ω denote a bounded domain with C^k boundary Γ. Then for any $1 \le l \le k$,

(i) there exists an open neighborhood N_k of 0 in

$$\Theta_k = \{\mathbf{V} \in C^k(\mathbb{R}^n,\mathbb{R}^n) : \text{derivatives of } \mathbf{V} \text{ up to order } k \text{ are bounded.}\} \quad (25)$$

and C^l functions $\Psi : N_k \to C^{k-l}(\Gamma)$ and $\Phi : N_k \to G^{k-l}(\Gamma,\Gamma)$ such that for any $\theta \in N_k$,

$$(I+\theta)\circ\Phi(\theta) = I + \Psi(\theta)\mathbf{n} \qquad \text{on } \Gamma. \quad (26)$$

(ii) Moreover, the values of the first- and second-order (Fréchet) derivatives of Ψ at $\theta = 0$ in the directions $\mathbf{V},\mathbf{W} \in \Theta_k$ are given by
  (a) $D_\theta\Psi(0)(\mathbf{V}) := \Psi'(0)(\mathbf{V}) = \mathbf{v}\cdot\mathbf{n}$ for $l \ge 1$, and
  (b) $D^2_\theta\Psi(0)(\mathbf{V},\mathbf{W}) := \Psi''(0)(\mathbf{V},\mathbf{W}) = -v_\Gamma \cdot D_\Gamma\mathbf{n}w_\Gamma - \mathbf{n}\cdot D_\Gamma\mathbf{v}w_\Gamma - \mathbf{n}\cdot D_\Gamma\mathbf{w}v_\Gamma$
  for $l \ge 2$, where $\mathbf{v} = \mathbf{V}|_\Gamma$ and $\mathbf{w} = \mathbf{W}|_\Gamma$.

The proof of the Lemma uses the implicit function Theorem and is given in [29, p.372]. This Lemma is the fundamental tool in proving the following result on the structure of the shape derivatives. Here, O_k denotes the set of bounded C^k domains.

Theorem 2.21 (see [29]): Consider the shape functional $J : O_k \to \mathbb{R}$ and the functional $\mathbf{J} : \bar{\Theta}_k \to \mathbb{R}$ where

$$\bar{\Theta}_k := \{\theta \in \Theta_k : |\theta|_{C^k} < 1\}, \qquad \textit{and} \quad \mathbf{J}(\theta) = J(\Omega_\theta). \quad (27)$$

For $k \ge 1$, the following statements hold.

(i) If $\Omega \in O_{k+1}$ and $\mathbf{J}$ is differentiable at 0 in Θ_k, then there is a continuous linear map $l_1 : C^k(\Gamma) \to \mathbb{R}$ such that for any $\mathbf{V} \in \Theta_k$,

$$D_\theta\mathbf{J}(0)(\mathbf{V}) := \mathbf{J}'(0)(\mathbf{V}) = l_1(\mathbf{v}\cdot\mathbf{n}). \quad (28)$$

(ii) If $\Omega \in O_{k+1}$ and $\mathbf{J}$ is twice differentiable at 0 in Θ_k then there exists a continuous bilinear symmetric map $l_2 : C^k(\Gamma)\times C^k(\Gamma) \to \mathbb{R}$ such that for any $\mathbf{V},\mathbf{W} \in \Theta_{k+1}$ we have

$$\begin{aligned} &D^2_\theta\mathbf{J}(0)(\mathbf{V},\mathbf{W}) := \mathbf{J}''(0)(\mathbf{V},\mathbf{W}) \\ &= l_2(\mathbf{v}\cdot\mathbf{n},\mathbf{w}\cdot\mathbf{n}) \\ &-l_1(v_\Gamma\cdot D_\Gamma\mathbf{n}w_\Gamma + \mathbf{n}\cdot D_\Gamma\mathbf{v}w_\Gamma + \mathbf{n}\cdot D_\Gamma\mathbf{w}v_\Gamma). \end{aligned} \quad (29)$$

Here, $\mathbf{v}$ and $\mathbf{w}$ are restrictions of $\mathbf{V}$ and $\mathbf{W}$ on Γ, respectively.

It is then shown that $d^2J(\Omega;\mathbf{V},\mathbf{W})$ can be written as (cf. [29]):

$$d^2J(\Omega;\mathbf{V},\mathbf{W}) = \mathbf{J}''(0)(\mathbf{V},\mathbf{W}) + \mathbf{J}'(0)(D\mathbf{V}\mathbf{W}). \quad (30)$$

where J'' and J' are the shape derivatives defined in (29) and (28), respectively.

III. Main Results

We now present the shape derivative methods that we used in obtaining the second-order Eulerian derivative $d^2J(\Omega;\mathbf{V},\mathbf{W})$ of the Kohn-Vogelius functional J. Throughout this section, we assume that the domains, deformation vectors, the state variables and the the rest of the functions involved to be regular enough. We first compute the material and shape derivatives of $\mathbf{n}$, τ and κ. Using these, together with the material and shape derivatives of the states u_D and u_N, the tools given in Section II and Steklov-Poincaré operators, we derive the $d^2J(\Omega;\mathbf{V},\mathbf{W})$.

In the discussion, we let $\mathbf{v} = \mathbf{V}|_\Sigma$ and $\mathbf{v} = \mathbf{v}_{\boldsymbol{\Sigma}} + v_n\mathbf{n}$. The scalar $v_n := \mathbf{v}\cdot\mathbf{n}$ is referred to as the normal component of $\mathbf{v}$ while the vector $\mathbf{v}_{\boldsymbol{\Sigma}}$ is its tangential component. In fact, $\mathbf{v}_{\boldsymbol{\Sigma}} = (\mathbf{v}\cdot\tau)\tau$. Also, we Remark that for a given scalar function f and vector function $\mathbf{V}$ defined on the free boundary Σ, the gradient ∇f, the Jacobian $D\mathbf{V}$ and divergence $\operatorname{div}\mathbf{V}$ refer actually to the gradient, Jacobian, and divergence of their respective extensions defined on a neighborhood of Σ.

A. Material and shape derivatives of $\mathbf{n}$, κ and τ

1) The material and shape derivative of $\mathbf{n}$*:* Let T_s be defined as in (6) but in the direction $\mathbf{W}$, not necessarily the same as $\mathbf{V}$. On the set Σ_s, where Σ_s is the free boundary of the perturbed domain Ω_s, the unit outward normal vector is denoted by $\mathbf{n}_s$ and is given by the following expression (see [11, p.358]):

$$\mathbf{n}_s = \frac{(DT_s)^{-T}\mathbf{n}}{|(DT_s)^{-T}\mathbf{n}|}\circ T_s^{-1}. \quad (31)$$

Theorem 3.1: The material derivative $\dot{\mathbf{n}}_W$ and shape derivative $\mathbf{n}'_W$ of the outward unit normal vector $\mathbf{n}$ at the boundary Σ in the direction of the deformation field $\mathbf{W}$ are given by

$$(i) \quad \dot{\mathbf{n}}_W = (D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}, \quad (32)$$

$$(ii) \quad \mathbf{n}'_W = (D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n} - (D\mathbf{n})\mathbf{W}. \quad (33)$$

Proof: Differentiating (31) at $s = 0$ we get the expression

$$\begin{aligned}\dot{\mathbf{n}}_W &:= \frac{\partial}{\partial s}(\mathbf{n}_s \circ T_s)\Big|_{s=0} \\ &= \frac{\frac{\partial}{\partial s}((DT_s)^{-T}\mathbf{n})|(DT_s)^{-T}\mathbf{n}|}{|(DT_s)^{-T}\mathbf{n}|^2}\Bigg|_{s=0} \\ &- \frac{\left[\frac{(DT_s)^{-T}\mathbf{n}}{|(DT_s)^{-T}\mathbf{n}|}\cdot\frac{\partial}{\partial s}((DT_s)^{-T}\mathbf{n})\right](DT_s)^{-T}\mathbf{n}}{|(DT_s)^{-T}\mathbf{n}|^2}\Bigg|_{s=0}.\end{aligned}$$

Simplifying we have

$$\begin{aligned}\dot{\mathbf{n}}_W &= \frac{[(-D\mathbf{W})^T\mathbf{n}]|\mathbf{n}| - \left(\frac{\mathbf{n}}{|\mathbf{n}|}\cdot\left[(-D\mathbf{W})^T\mathbf{n}\right]\right)\mathbf{n}}{|\mathbf{n}|^2} \\ &= -(D\mathbf{W})^T\mathbf{n} + (\mathbf{n}\cdot(D\mathbf{W})^T\mathbf{n})\mathbf{n} \\ &= (D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}.\end{aligned}$$

Applying (13) we get $\mathbf{n}'_W = (D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n} - (D\mathbf{n})\mathbf{W}$. ■

2) The material and shape derivative of κ: The computation of the material derivative of the mean curvature of Σ requires the concept of unitary extension of $\mathbf{n}$. We say that $\mathbf{N}$ is the unitary extension of $\mathbf{n}$ on Σ if $\mathbf{N}\cdot\mathbf{N} = 1$ in a neighborhood of Σ. This extension has the following property:

Lemma 3.2 (see [32]): If $\mathbf{N} \in C^1(\mathbb{R}^n, \mathbb{R}^n)$ then $(D\mathbf{N})^T\mathbf{n} = 0$ on Σ.

Definition 3.3 (see [11]): The *mean curvature* κ of an $(n-1)$-dimensional manifold Γ is defined as

$$\kappa = \frac{1}{n-1}\operatorname{div}_\Gamma \mathbf{n}.$$

For $n = 2$, this is simply the curvature, and it is given by $\kappa = \operatorname{div}_\Sigma \mathbf{n}$.

The derivation for the expression $\dot{\kappa}_W$ utilizes the transported divergence.

Lemma 3.4 (see [32]): Let $\mathbf{v}$ be a C^k vector field in $\mathbb{R}^n$ and $T_t : \bar{U} \subset \mathbb{R}^n \to \mathbb{R}^n$ be a C^k transformation. Then $(\operatorname{div}\mathbf{v})\circ T_t \in C^{k-1}(U, \mathbb{R}^n)$ and is given by

$$(\operatorname{div}\mathbf{v})\circ T_t = \operatorname{Tr}[D(\mathbf{v}\circ T_t)(DT_t)^{-1}].$$

So if $\mathbf{N}_s$ is a smooth extension of the normal field $\mathbf{n}_s$ on a neighborhood of Σ_s, then by applying Lemma 3.4 we have

$$(\operatorname{div}\mathbf{N}_s)\circ T_s = \operatorname{Tr}[D(\mathbf{N}_s\circ T_s)(DT_s)^{-1}], \tag{34}$$

and if $\mathbf{N}$ is a unitary extension of $\mathbf{n}$ on a neighborhood of Σ, we get $\operatorname{div}\mathbf{N} = \operatorname{Tr}(D\mathbf{N})$, which can be justified to be the curvature κ because

$$\kappa = \operatorname{div}_\Sigma \mathbf{n} = (\operatorname{div}\mathbf{N}) - (D\mathbf{N})\mathbf{n}\cdot\mathbf{n}$$

and $\mathbf{n}^T D\mathbf{N} = 0$ on the boundary as supported by Lemma 3.2.

Theorem 3.5: The material derivative $\dot{\kappa}_W$ and shape derivative κ'_W of the mean curvature κ of the boundary Σ in the direction of the deformation field $\mathbf{W}$ are given by

$$\begin{aligned}(i)\quad \dot{\kappa}_W &= \operatorname{Tr}\Big[D\Big((D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}\Big) \\ &\qquad - D\mathbf{n}D\mathbf{W}\Big]\end{aligned} \tag{35}$$

$$\begin{aligned}(ii)\quad \kappa'_W &= \operatorname{Tr}\Big[D\Big((D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}\Big) \\ &\qquad - D\mathbf{n}D\mathbf{W}\Big] - \nabla\kappa\cdot\mathbf{W}.\end{aligned} \tag{36}$$

Proof: The mean curvature κ_s of the manifold Σ_s is given by

$$\kappa_s = \operatorname{div}_{\Sigma_s}\mathbf{n}_s = (\operatorname{div}\mathbf{N}_s) - (D\mathbf{N}_s)\mathbf{n}_s\cdot\mathbf{n}_s,$$

for any arbitrary smooth extension $\mathbf{N}_s$ of $\mathbf{n}_s$ on the neighborhood of Σ_s, and if $\mathbf{N}_s$ is a unitary extension of $\mathbf{n}_s$, then by Lemma 3.2 we have

$$\kappa_s = \operatorname{div}\mathbf{N}_s.$$

So for a unitary extension $\mathbf{N}_s$ we write $\kappa_s\circ T_s$ as

$$\kappa_s\circ T_s = (\operatorname{div}\mathbf{N}_s)\circ T_s = \operatorname{Tr}[D(\mathbf{N}_s\circ T_s)(DT_s)^{-1}].$$

Therefore, applying Lemma 2.4 and (32), the explicit form of the material derivative of the mean curvature κ in the direction $\mathbf{W}$ is obtained as follows:

$$\begin{aligned}\dot{\kappa}_W &= \frac{\partial}{\partial s}(\kappa_s\circ T_s)\Big|_{s=0} \\ &= \operatorname{Tr}\left[\left(\frac{\partial}{\partial s}D(\mathbf{N}_s\circ T_s)\right)(DT_s)^{-1} \right.\\ &\qquad \left.+ (D\mathbf{N}_s)\circ T_s\left(\frac{\partial}{\partial s}(DT_s)^{-1}\right)\right]\Bigg|_{s=0} \\ &= \operatorname{Tr}[D\dot{\mathbf{n}}_W - D\mathbf{n}D\mathbf{W}] \\ &= \operatorname{Tr}\Big[D\Big((D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}\Big) - D\mathbf{n}D\mathbf{W}\Big].\end{aligned} \tag{37}$$

Thus, the shape derivative of κ is given by (36). ■

3) The material and shape derivative of τ: The unit tangent vector on Σ is represented by τ. It is oriented in such a way that Σ is at the left of τ; that is, if $\mathbf{n} = (n_1, n_2)^T$ then we represent $\tau = (-n_2, n_1)^T$.

Theorem 3.6: The material derivative $\dot{\tau}_W$ and shape derivative τ'_W of the unit tangent vector τ on the boundary Σ in the direction of the deformation field $\mathbf{W}$ are given by

$$(i)\quad \dot{\tau}_W = [(D\mathbf{W})^T\mathbf{n}\cdot\tau]\mathbf{n}, \tag{38}$$

$$(ii)\quad \tau'_W = [(D\mathbf{W})^T\mathbf{n}\cdot\tau]\mathbf{n} - (D\tau)\mathbf{W}. \tag{39}$$

Proof: Since $\mathbf{n}$ and τ are orthogonal to each other, we derive the material and shape derivatives of τ by determining the material derivative of $\mathbf{n}\cdot\tau = 0$ in the direction $\mathbf{W}$. First, we get the identity $\dot{\mathbf{n}}_W\cdot\tau + \mathbf{n}\cdot\dot{\tau}_W = 0$. Applying (32) we obtain

$$\big((D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}\big)\cdot\tau + \mathbf{n}\cdot\dot{\tau}_W = 0,$$

which can be simplified into

$$-(D\mathbf{W})^T\mathbf{n}\cdot\tau + \mathbf{n}\cdot\dot{\tau}_W = 0.$$

Therefore, we get (i) since $\dot{\tau}\cdot\tau = 0$. By applying the Definition of shape derivative, we obtain (ii). ■

B. Differentiation Approach of Sokolowski and Zolesio

Let us recall the first-order Eulerian derivative of the Kohn-Vogelius cost functional J (cf. [1], [4], [5]):

Theorem 3.7: For $C^{1,1}$ bounded domain Ω, the first-order shape derivative of the Kohn-Vogelius cost functional

$$J(\Omega) = \frac{1}{2}\int_{\Omega} |\nabla(u_D - u_N)|^2 \, \mathrm{d}x$$

in the direction of a perturbation field $\mathbf{V} \in \Theta$, where Θ is defined by (5) and the state functions u_D and u_N satisfy the Dirichlet problem (3) and the Neumann problem (4), respectively, is given by

$$dJ(\Omega;\mathbf{V}) = \frac{1}{2}\int_{\Sigma} (\lambda^2 - (\nabla u_D \cdot \mathbf{n})^2 + 2\lambda\kappa u_N - (\nabla u_N \cdot \tau)^2)\mathbf{V}\cdot\mathbf{n}\, \mathrm{d}s,$$

where $\mathbf{n}$ is the unit exterior normal vector to Σ, τ is a unit tangent vector to Σ, and κ is the mean curvature of Σ.

Now we will be computing the second-order Eulerian derivative of this functional by following the technique used by Sokolowski and Zolesio [32]. This technique bypasses the use of domain differentiation and boundary differentiation formulas. It highly involves, however, material and shape derivatives of states.

We first note that the derivative $dJ(\Omega_s(\mathbf{W});\mathbf{V})$ exists for all sufficiently small s. This follows from the result on the first-order Eulerian derivative given in [4].

By Definition, we write the second-order Eulerian derivative as follows.

$$\begin{aligned} d^2J(\Omega;\mathbf{V},\mathbf{W}) &= \lim_{s\to 0^+} \frac{dJ(\Omega_s(\mathbf{W}),\mathbf{V}) - dJ(\Omega;\mathbf{V})}{s} \\ &= \frac{\partial}{\partial s}\left\{\frac{\partial}{\partial t} J(\Omega_{t,s})\Big|_{t=0}\right\}\Big|_{s=0} \\ &= \frac{\partial}{\partial s}\left(\int_{\Sigma_s} F_s \mathbf{V}\cdot\mathbf{n}_s \, \mathrm{d}\Sigma_s\right)\Big|_{s=0}, \end{aligned} \tag{40}$$

where

$$F_s = \lambda^2 - (\nabla u_{D,s}\cdot\mathbf{n}_s)^2 + 2\lambda\kappa_s u_{N,s} - (\nabla u_{N,s}\cdot\tau_s)^2 \tag{41}$$

and the deformation fields $\mathbf{V}$ and $\mathbf{W}$ are assumed to belong in Θ defined by (5).

Remark 3.8: The expression for F_s has a coefficient of $\frac{1}{2}$. For the sake of simplicity we first disregard this coefficient and affix it in the final result.

Using the boundary transformation formula given in Lemma 2.10, we write (40) as

$$\begin{aligned} &d^2J(\Omega;\mathbf{V},\mathbf{W}) \\ &= \frac{\partial}{\partial s}\left(\int_{\Sigma} (F_s\circ T_s)[(\mathbf{V}\circ T_s)\cdot(\mathbf{n}_s\circ T_s)] w_s \, \mathrm{d}\Sigma\right)\Big|_{s=0} \end{aligned} \tag{42}$$

where w_s is defined by

$$w_s(x) = \det DT_s(x) |(DT_s)^{-T}\mathbf{n}(x)|, \text{ for any } x \in \Sigma. \tag{43}$$

Clearly, $(\mathbf{V}\circ T_s)\cdot(\mathbf{n}_s\circ T_s)|_{s=0} = \mathbf{V}\cdot\mathbf{n}$ and $(F_s \circ T_s)w_s|_{s=0} = F$, where

$$F = \lambda^2 - (\nabla u_D\cdot\mathbf{n})^2 + 2\lambda\kappa u_N - (\nabla u_N\cdot\tau)^2. \tag{44}$$

Therefore, we write (42) as

$$\begin{aligned} &d^2J(\Omega;\mathbf{V},\mathbf{W}) \\ &= \int_{\Sigma}\left[\frac{\partial}{\partial s}((F_s\circ T_s)w_s)\right]\Big|_{s=0} \mathbf{V}\cdot\mathbf{n}\,\mathrm{d}\Sigma \\ &\quad + \int_{\Sigma} F\left[\frac{\partial}{\partial s}\{(\mathbf{V}\circ T_s)\cdot(\mathbf{n}_s\circ T_s)\}\right]\Big|_{s=0} \mathrm{d}\Sigma. \end{aligned} \tag{45}$$

We first examine the expression $\frac{\partial}{\partial s}\{(\mathbf{V}\circ T_s)\cdot(\mathbf{n}_s\circ T_s)\}\Big|_{s=0}$. Applying Lemma 2.4 (property (7)), we can write this expressions as

$$\begin{aligned} &\frac{\partial}{\partial s}\{(\mathbf{V}\circ T_s)\cdot(\mathbf{n}_s\circ T_s)\}\Big|_{s=0} \\ &= (D\mathbf{V})\mathbf{W}\cdot\mathbf{n} + \mathbf{V}\cdot\frac{\partial}{\partial s}(\mathbf{n}_s\circ T_s)\Big|_{s=0}. \end{aligned} \tag{46}$$

Applying (32), one can write (46) as

$$\begin{aligned} &\frac{\partial}{\partial s}\{(\mathbf{V}\circ T_s)\cdot(\mathbf{n}_s\circ T_s)\}\Big|_{s=0} \\ &= (D\mathbf{V})\mathbf{W}\cdot\mathbf{n} + \mathbf{V}\cdot[(D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}] \end{aligned} \tag{47}$$

Next we turn to the discussion of the derivative of $(F_s \circ T_s)w_s$.

$$\begin{aligned} &\frac{\partial}{\partial s}\Big((F_s\circ T_s)w_s\Big)\Big|_{s=0} \\ &= \left\{\left(\frac{\partial}{\partial s}(F_s\circ T_s)\right)w_s + (F_s\circ T_s)\frac{\partial}{\partial s}w_s\right\}\Big|_{s=0} \end{aligned} \tag{48}$$

Since

$$\begin{aligned} F_s\circ T_s &= \lambda^2 - ((\nabla u_{D,s}\circ T_s)\cdot(\mathbf{n}_s\circ T_s))^2 \\ &+ 2\lambda(\kappa_s\circ T_s)(u_{N,s}\circ T_s) - [(\nabla u_{N,s}\circ T_s)\cdot(\tau_s\circ T_s)]^2, \end{aligned}$$

one finds

$$\begin{aligned} &\frac{\partial}{\partial s}(F_s\circ T_s)\Big|_{s=0} \\ &= -2\frac{\partial u_D}{\partial\mathbf{n}}\frac{\partial}{\partial s}\left[(DT_s)^{-T}\nabla(u_{D,s}\circ T_s)\cdot(\mathbf{n}_s\circ T_s)\right]\Big|_{s=0} \\ &\quad + 2\lambda\frac{\partial}{\partial s}((\kappa_s\circ T_s)(u_{N,s}\circ T_s))\Big|_{s=0} \\ &\quad - 2\frac{\partial u_N}{\partial\tau}\frac{\partial}{\partial s}\left((DT_s)^{-T}\nabla(u_{N,s}\circ T_s)\cdot(\tau_s\circ T_s)\right)\Big|_{s=0} \\ &=: Q_1 + Q_2 + Q_3. \end{aligned}$$

We simplify these three terms, starting off with the expression Q_1. We use Property 10 of Lemma 2.4 and (32) to obtain:

$$\begin{aligned} Q_1 &= -2\frac{\partial u_D}{\partial\mathbf{n}}\Big\{\Big[(-D\mathbf{W})^T\nabla u_D \\ &\qquad + \nabla\Big[\frac{\partial}{\partial s}(u_{D,s}\circ T_s)\Big|_{s=0}\Big]\Big]\cdot\mathbf{n}\Big\} \\ &\quad - 2\frac{\partial u_D}{\partial\mathbf{n}}\left\{\nabla u_D\cdot\left[(D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}\right]\right\} \end{aligned}$$

Noting that $u_D = 0$ on Σ, we have $\nabla u_D = \dfrac{\partial u_D}{\partial\mathbf{n}}\mathbf{n}$ on Σ. Thus, the expression

$\nabla u_D \cdot \big[(D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}\big]$ vanishes. Therefore, Q_1 can be simplified to

$$\begin{aligned} Q_1 &= -2\frac{\partial u_D}{\partial \mathbf{n}}\left\{-(D\mathbf{W})^T\nabla u_D\cdot\mathbf{n}\right. \\ &\qquad \left. +\nabla \dot{u}_{D,W}\cdot\mathbf{n}\right\} \\ &= -2\frac{\partial u_D}{\partial \mathbf{n}}\left\{-(D\mathbf{W})^T\nabla u_D\cdot\mathbf{n} + \nabla u'_{D,W}\cdot\mathbf{n}\right. \\ &\qquad \left. +\nabla(\nabla u_D\cdot\mathbf{W})\cdot\mathbf{n}\right\}, \end{aligned} \tag{49}$$

where the shape derivative $u'_{D,W}$ can be shown to satisfy the following boundary value problem:

$$\begin{cases} -\Delta u'_{D,W} &= 0 \quad \text{in } \Omega, \\ u'_{D,W} &= 0 \quad \text{on } \Gamma, \\ u'_{D,W} &= -\mathbf{W}\cdot\mathbf{n}\dfrac{\partial u_D}{\partial \mathbf{n}} \quad \text{on } \Sigma. \end{cases} \tag{50}$$

Next we simplify Q_2 as follows.

$$\begin{aligned} Q_2 &= 2\lambda\frac{\partial}{\partial s}\left[(\kappa_s\circ T_s)(u_{N,s}\circ T_s)\right]\bigg|_{s=0} \\ &= 2\lambda\left[\dot{\kappa}_W u_N + \kappa(u'_{N,W} + \nabla u_N\cdot\mathbf{W})\right] \end{aligned} \tag{51}$$

where $\dot{\kappa}_W$ is given by (35) and $u'_{N,W}$ may be shown to satisfy the following boundary value problem:

$$\begin{cases} -\Delta u'_{N,W} &= 0 \quad \text{in } \Omega, \\ u'_{N,W} &= 0 \quad \text{on } \Gamma, \\ \dfrac{\partial u'_{N,W}}{\partial \mathbf{n}} &= \operatorname{div}_\Sigma(\mathbf{W}\cdot\mathbf{n}\nabla_\Sigma u_N) + \mathbf{W}\cdot\mathbf{n}\kappa\lambda \quad \text{on } \Sigma. \end{cases} \tag{52}$$

Similar to what we did for the expression Q_1, we simplify Q_3 as follows:

$$\begin{aligned} Q_3 &= -2\frac{\partial u_N}{\partial \tau}\left[(-D\mathbf{W})^T\nabla u_N\cdot\tau + \nabla u'_{N,W}\cdot\tau\right. \\ &\qquad \left. +\nabla(\nabla u_N\cdot\mathbf{W})\cdot\tau + \nabla u_N\cdot\dot{\tau}_W\right], \end{aligned} \tag{53}$$

where $\dot{\tau}_W$ is given by (39). Combining (49), (51), and (53), we obtain the material derivative of F at Σ in the direction $\mathbf{W}$:

$$\begin{aligned} \dot{F}_W &:= \frac{\partial}{\partial s}(F_s\circ T_s)\bigg|_{s=0} \\ &= -2\frac{\partial u_D}{\partial \mathbf{n}}\left\{-(D\mathbf{W})^T\nabla u_D\cdot\mathbf{n} + \nabla u'_{D,W}\cdot\mathbf{n}\right\} \\ &\quad -2\frac{\partial u_D}{\partial \mathbf{n}}\left\{\nabla(\nabla u_D\cdot\mathbf{W})\cdot\mathbf{n}\right\} \\ &\quad +2\lambda[\dot{\kappa}_W u_N + \kappa(u'_{N,W} + \nabla u_N\cdot\mathbf{W})] \\ &\quad -2\frac{\partial u_N}{\partial \tau}\left[(-D\mathbf{W})^T\nabla u_N\cdot\tau + \nabla u'_{N,W}\cdot\tau\right] \\ &\quad -2\frac{\partial u_N}{\partial \tau}\left[\nabla(\nabla u_N\cdot\mathbf{W})\cdot\tau + \nabla u_N\cdot\dot{\tau}_W\right], \end{aligned} \tag{54}$$

where $\dot{\kappa}_W$ and $\dot{\tau}_W$ are given by (35) and (39), respectively.

Next we express $\dot{F}_W$ in terms of the shape derivatives of κ and τ, and of states u_D and u_N in the direction $\mathbf{W}$ by using the identity:

$$-(D\mathbf{W})^T\nabla u_D\cdot\mathbf{n} + \nabla(\nabla u_D\cdot\mathbf{W})\cdot\mathbf{n} = (\nabla^2 u_D)\mathbf{W}\cdot\mathbf{n}. \tag{55}$$

This identity is derived by expanding $\nabla(\nabla u_D\cdot\mathbf{W})\cdot\mathbf{n}$ as follows:

$$\begin{aligned} &\nabla(\nabla u_D\cdot\mathbf{W})\cdot\mathbf{n} \\ &= \left\{[D(\nabla u_D)]^T\mathbf{W} + (D\mathbf{W})^T\nabla u_D\right\}\cdot\mathbf{n} \\ &= [D(\nabla u_D)]^T\mathbf{W}\cdot\mathbf{n} + (D\mathbf{W})^T\nabla u_D\cdot\mathbf{n}, \end{aligned}$$

and by replacing $[D(\nabla u_D)]^T$ with the Hessian $\nabla^2 u_D$, which is symmetric for $u_D \in H^2(\Omega)$. Similarly, the following identity is valid.

$$-(D\mathbf{W})^T\nabla u_N\cdot\tau + \nabla(\nabla u_N\cdot\mathbf{W})\cdot\tau = (\nabla^2 u_N)\mathbf{W}\cdot\tau. \tag{56}$$

Using the identity $\dot{\kappa}_W = \kappa'_W + \nabla\kappa\cdot\mathbf{W}$ and the equations (55) and (56) into (54), we can now write $\dot{F}_W$ as

$$\begin{aligned} \dot{F}_W &= -2\frac{\partial u_D}{\partial \mathbf{n}}(\nabla u'_{D.W}\cdot\mathbf{n} + (\nabla^2 u_D)\mathbf{W}\cdot\mathbf{n}) \\ &\quad +2\lambda(\kappa'_W + \nabla\kappa\cdot\mathbf{W})u_N + \kappa(u'_{N,W} + \nabla u_N\cdot\mathbf{W}) \\ &\quad -2(\nabla u_N\cdot\tau)(\nabla u'_{N,W}\cdot\tau \\ &\quad +(\nabla^2 u_N)\mathbf{W}\cdot\tau + \nabla u_N\cdot(\tau'_W + (D\tau)\mathbf{W})), \end{aligned} \tag{57}$$

where the shape derivatives $u'_{D,W}$ and $u'_{N,W}$ satisfy the boundary value problems (50) and (52), respectively, τ'_W is given by (39), and κ'_W is given by (36).

Also, the following equation holds because of Lemma 2.4:

$$\frac{\partial}{\partial s}\Big((F_s\circ T_s)w_s\Big)\bigg|_{s=0} = \dot{F}_W + F\operatorname{div}_\Sigma\mathbf{W}, \tag{58}$$

where $\dot{F}_W$ and F are given by (57) and (44), respectively. By substituting equations (58) and (47) into (45), we can write $d^2J(\Omega;\mathbf{V};\mathbf{W})$ as $d^2J(\Omega;\mathbf{V};\mathbf{W})$

$$\begin{aligned} &d^2J(\Omega;\mathbf{V};\mathbf{W}) \\ &= \int_\Sigma\left[\dot{F}_W + F\operatorname{div}_\Sigma\mathbf{W}\right]\mathbf{V}\cdot\mathbf{n}\,d\Sigma \\ &+ \int_\Sigma F\Big[(D\mathbf{V})\mathbf{W}\cdot\mathbf{n} + (D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{V}\cdot\mathbf{n} \\ &- (D\mathbf{W})\mathbf{V}\cdot\mathbf{n}\Big]\,d\Sigma. \end{aligned} \tag{59}$$

1) The symmetric and nonsymmetric parts of $d^2J(\Omega;\mathbf{V},\mathbf{W})$: We first rewrite (59) as follows:

$$\begin{aligned} d^2J(\Omega;\mathbf{V},\mathbf{W}) &= \int_\Sigma \dot{F}_W\mathbf{V}\cdot\mathbf{n}\,d\Sigma \\ &+ \int_\Sigma F(\operatorname{div}_\Sigma\mathbf{W})\mathbf{V}\cdot\mathbf{n}\,d\Sigma \\ &+ \int_\Sigma F[(D\mathbf{V})\mathbf{W}\cdot\mathbf{n} + (D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{V}\cdot\mathbf{n} \\ &\quad -(D\mathbf{W})\mathbf{V}\cdot\mathbf{n}]\,d\Sigma. \end{aligned}$$

Using the relationship $\dot{F}_W = F'_W + \nabla F\cdot\mathbf{W}$, the Definition of tangential gradient and tangential divergence, we write the second-order Eulerian derivative as follows:

$$\begin{aligned} d^2J(\Omega;\mathbf{V},\mathbf{W}) &= \int_\Sigma F'_W v_n\,d\Sigma \\ &+ \int_\Sigma \{[(\nabla_\Sigma F + (\nabla F\cdot\mathbf{n})\mathbf{n})\cdot\mathbf{W}]v_n\,d\Sigma \\ &+ F(\operatorname{div}_\Sigma\mathbf{W} + D\mathbf{W}\mathbf{n}\cdot\mathbf{n})v_n - F(D\mathbf{W})\mathbf{V}\cdot\mathbf{n}\}\,d\Sigma \\ &+ \int_\Sigma F(D\mathbf{V})\mathbf{W}\cdot\mathbf{n}\,d\Sigma \\ &=: I_1 + I_2 + I_3. \end{aligned}$$

We skip I_1 and I_3 and proceed to simplify I_2. First we observe that

$$\nabla_\Sigma v_n \cdot \mathbf{n} = 0, \qquad (60)$$

where v_n is the normal component of $\mathbf{V}$ restricted to Σ. Second, we also observe that

$$\kappa v_n = \mathrm{div}_\Sigma(v_n \mathbf{n}). \qquad (61)$$

This follows from $\mathrm{div}_\Sigma(v_n\mathbf{n}) = \nabla_\Sigma v_n \cdot \mathbf{n} + v_n \,\mathrm{div}_\Sigma\, \mathbf{n}$, (60), and the Definition of curvature.

Then we consider the following Lemma (cf. [11]):

Lemma 3.9: Let $\mathbf{V}$ and $\mathbf{W}$ be smooth deformation fields on a neighborhood of Σ and $\mathbf{v} = \mathbf{V}|_\Sigma$ and $\mathbf{w} = \mathbf{W}|_\Sigma$. Then the following equalities hold:

$$(i) \quad \mathbf{v_\Sigma} \cdot \nabla_\Sigma w_n = \mathbf{n} \cdot (D_\Sigma \mathbf{w})\mathbf{v_\Sigma} + v_\Sigma \cdot D\mathbf{n}\mathbf{w_\Sigma}, \qquad (62)$$

$$\begin{aligned}(ii) \quad (D\mathbf{V})\mathbf{W}\cdot\mathbf{n} &= \mathbf{w_\Sigma} \cdot (\nabla_\Sigma v_n - (D\mathbf{n})\mathbf{v_\Sigma}) \\ &\quad + D\mathbf{V}\mathbf{n}\cdot\mathbf{n} w_n.\end{aligned} \qquad (63)$$

Applying property (ii) of Lemma 3.9 we obtain

$$(D\mathbf{W})\mathbf{V}\cdot\mathbf{n} = \mathbf{v_\Sigma}\cdot(\nabla_\Sigma w_n - (D\mathbf{n})\mathbf{w_\Sigma}) + D\mathbf{W}\mathbf{n}\cdot\mathbf{n} v_n. \quad (64)$$

Using (64), we write I_2 as

$$\begin{aligned} I_2 &= \int_\Sigma \left[\frac{\partial F}{\partial \mathbf{n}} w_n v_n + (\nabla_\Sigma F \cdot \mathbf{W}) v_n + F(\mathrm{div}_\Sigma\, \mathbf{W}) v_n \right. \\ &\quad \left. - \Big(\mathbf{v_\Sigma} \cdot (\nabla_\Sigma w_n - (D\mathbf{n})\mathbf{w_\Sigma}) \Big) \right] \mathrm{d}\Sigma. \end{aligned}$$

By adding and subtracting $F\mathbf{w_\Sigma} \cdot \nabla_\Sigma v_n$, we have

$$\begin{aligned} I_2 &= \int_\Sigma \frac{\partial F}{\partial \mathbf{n}} w_n v_n + (\nabla_\Sigma F \cdot \mathbf{W}) v_n + F(\mathrm{div}_\Sigma\, \mathbf{W}) v_n \,\mathrm{d}\Sigma \\ &+ \int_\Sigma F \mathbf{w_\Sigma} \cdot \nabla_\Sigma v_n \,\mathrm{d}\Sigma \\ &- \int_\Sigma F(\mathbf{v_\Sigma} \cdot \nabla_\Sigma w_n - \mathbf{v_\Sigma} \cdot D\mathbf{n}\mathbf{w_\Sigma} + \mathbf{w_\Sigma} \cdot \nabla_\Sigma v_n) \,\mathrm{d}\Sigma. \end{aligned}$$

From Lemma 3.9, we obtain the following identities:

$$\begin{aligned} \mathbf{v_\Sigma} \cdot \nabla_\Sigma w_n &= \mathbf{n} \cdot (D_\Sigma \mathbf{w}) \mathbf{v_\Sigma} + v_\Sigma \cdot D\mathbf{n}\mathbf{w_\Sigma} \quad \text{and} \\ \mathbf{w_\Sigma} \cdot \nabla_\Sigma v_n &= \mathbf{n} \cdot (D_\Sigma \mathbf{v}) \mathbf{w_\Sigma} + \mathbf{w_\Sigma} \cdot D\mathbf{n}\mathbf{v_\Sigma}. \end{aligned} \qquad (65)$$

Using these identities and because $D\mathbf{n} = D_\Sigma\mathbf{n} + ((D\mathbf{n})\mathbf{n})\cdot\mathbf{n} = D_\Sigma \mathbf{n}$ on Σ we can now write I_2 as

$$\begin{aligned} I_2 &= \int_\Sigma \Big\{ \frac{\partial F}{\partial \mathbf{n}} v_n w_n + (\nabla_\Sigma F \cdot \mathbf{W}) v_n + F(\mathrm{div}_\Sigma\, \mathbf{W}) v_n \\ &\qquad + F\mathbf{w_\Sigma} \cdot \nabla_\Sigma v_n \Big\} \,\mathrm{d}\Sigma \\ &\quad - \int_\Sigma F\big(\mathbf{v_\Sigma} \cdot D_\Sigma \mathbf{n}\mathbf{w_\Sigma} + \mathbf{n} \cdot D_\Sigma \mathbf{v}\mathbf{w_\Sigma} \\ &\qquad + \mathbf{n} \cdot D_\Sigma \mathbf{w}\mathbf{v_\Sigma}\big) \,\mathrm{d}\Sigma \\ &=: I_{21} + I_{22}. \end{aligned}$$

We retain I_{22} and simplify I_{21}. Here we first decompose $\mathbf{W}$ in terms of its tangential and normal components. Then we use (61) to obtain the following:

$$\begin{aligned} I_{21} &= \int_\Sigma \left(\frac{\partial F}{\partial \mathbf{n}} v_n w_n + \kappa F v_n w_n \right) \mathrm{d}\Sigma \\ &\quad + \int_\Sigma \Big\{ (\nabla_\Sigma F \cdot \mathbf{W}) v_n + F(\mathrm{div}_\Sigma\, \mathbf{w_\Sigma}) v_n \\ &\qquad + F\mathbf{w_\Sigma} \cdot \nabla_\Sigma v_n \Big\} \,\mathrm{d}\Sigma. \end{aligned}$$

The second integral of I_{21} may be shown to vanish. Thus I_{21} becomes

$$I_{21} = \int_\Sigma \left(\frac{\partial F}{\partial \mathbf{n}} + \kappa F \right) v_n w_n. \qquad (66)$$

Consequently, we write I_2 as

$$\begin{aligned} I_2 &= \int_\Sigma \left(\frac{\partial F}{\partial \mathbf{n}} + \kappa F \right) v_n w_n \,\mathrm{d}\Sigma \\ &\quad - \int_\Sigma F \Big(\mathbf{v_\Sigma} \cdot D_\Sigma \mathbf{n}\mathbf{w_\Sigma} + \mathbf{n} \cdot D_\Sigma \mathbf{v}\mathbf{w_\Sigma} \\ &\qquad + \mathbf{n} \cdot D_\Sigma \mathbf{w}\mathbf{v_\Sigma} \Big) \,\mathrm{d}\Sigma. \end{aligned} \qquad (67)$$

Therefore, by considering (67) and incorporating the constant $\frac{1}{2}$ that we have neglected at the start of derivation, we obtain a nice structure for $d^2 J(\Omega; \mathbf{V}, \mathbf{W})$:

$$\begin{aligned} & d^2 J(\Omega; \mathbf{V}, \mathbf{W}) \\ &= \frac{1}{2} \int_\Sigma \Big[F'_W v_n + \left(\frac{\partial F}{\partial \mathbf{n}} + \kappa F \right) v_n w_n \\ &\quad - F(\mathbf{v_\Sigma} \cdot D_\Sigma \mathbf{n}\mathbf{w_\Sigma} + \mathbf{n} \cdot D_\Sigma \mathbf{v}\mathbf{w_\Sigma} + \mathbf{n} \cdot D_\Sigma \mathbf{w}\mathbf{v_\Sigma}) \Big] \,\mathrm{d}\Sigma \\ &\quad + \frac{1}{2} \int_\Sigma F(D\mathbf{V})\mathbf{W} \cdot \mathbf{n} \,\mathrm{d}\Sigma, \end{aligned} \qquad (68)$$

where F is given by (44) and F'_W by

$$\begin{aligned} F'_W &= \frac{\partial}{\partial s} F_s \Big|_{s=0} \\ &= -2 \frac{\partial u_D}{\partial \mathbf{n}} [\nabla u'_{D,W} \cdot \mathbf{n} + \nabla u_D \cdot \mathbf{n}'_W] \\ &\quad + 2\lambda(\kappa'_W u_N + \kappa u'_{N,W}) \\ &\quad - 2 \frac{\partial u_N}{\partial \tau} [\nabla u'_{N,W} \cdot \tau + \nabla u_N \cdot \tau'_W]. \end{aligned} \qquad (69)$$

The first and second integrals of (68) are the symmetric and nonsymmetric parts of the second-order Eulerian derivative of J, respectively. Our results satisfy the structure given by Novruzi and Pierre (see subsection II-B).

C. The domain differentiation approach

To further validate our result, we present in this subsection an alternative method to derive to the second-order Eulerian derivative of J. This time we use a domain differentiation approach. As before, we start with

$$d^2 J(\Omega; \mathbf{V}, \mathbf{W}) = \frac{1}{2} \frac{\partial}{\partial s} \int_{\Sigma_s(\mathbf{W})} (F_s \mathbf{V} \cdot \mathbf{n}_s \,\mathrm{d}\Sigma_s) \Big|_{s=0},$$

where F_s is given by (41). Here $u_{D,s}$ and $u_{N,s}$ satisfy (50), and (52), respectively; $\kappa_s = \mathrm{div}_{\Sigma_s}\, \mathbf{n}_s$; and $\mathbf{n}_s$ and τ_s refer to the unit outward normal and unit tangent vectors on Σ_s, respectively. Using Stoke's theorem we first transform the boundary integral into a domain integral then apply the domain differentiation formula (21) to get

$$\begin{aligned} 2d^2 J(\Omega; \mathbf{V}, \mathbf{W}) &= \frac{\partial}{\partial s} \int_{\Sigma_s(\mathbf{W})} (F_s \mathbf{V} \cdot \mathbf{n}_s \,\mathrm{d}\Sigma_s) \Big|_{s=0} \\ &= \frac{\partial}{\partial s} \int_{\Omega_s(\mathbf{W})} \mathrm{div}(F_s \mathbf{V}) \,\mathrm{d}x \Big|_{s=0} \\ &= \int_\Omega \left\{ \frac{\partial}{\partial s} \mathrm{div}(F_s \mathbf{V}) + \mathrm{div}\left[(\mathrm{div}(F_s \mathbf{V})) \mathbf{W} \right] \right\} \Big|_{s=0} \mathrm{d}x \end{aligned}$$

Applying Stoke's formula again, we find

$$2d^2J(\Omega;\mathbf{V},\mathbf{W}) = \int_\Omega \operatorname{div}\Big[F'_W\mathbf{V} + [\operatorname{div}(F\mathbf{V})]\mathbf{W}\Big]\,\mathrm{d}x$$
$$= \int_\Sigma \Big\{F'_W\mathbf{V}\cdot\mathbf{n} + [\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\Big\}\,\mathrm{d}\Sigma,$$

where F'_W is given by (69).

As before, we write $\mathbf{v}$ in terms of its normal and tangential components. Applying the divergence, tangential gradient and tangential divergence formulas given in Lemma 2.15, we can write $\int_\Sigma[\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma$ as follows:

$$\int_\Sigma[\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma = \int_\Sigma[\operatorname{div}(F\mathbf{V})]w_n\,\mathrm{d}\Sigma$$
$$= \int_\Sigma[(\nabla F)\cdot\mathbf{v} + F\operatorname{div}\mathbf{V}]w_n\,\mathrm{d}\Sigma$$
$$= \int_\Sigma\Big\{\Big(\nabla_\Sigma F + (\nabla F\cdot\mathbf{n})\mathbf{n}\Big)\cdot(\mathbf{v_\Sigma} + v_n\mathbf{n})$$
$$+F(\operatorname{div}_\Sigma\mathbf{v} + D\mathbf{V}\mathbf{n}\cdot\mathbf{n})\Big\}w_n\,\mathrm{d}\Sigma$$
$$= \int_\Sigma\Big\{(\nabla_\Sigma F)\cdot\mathbf{v_\Sigma} + (\nabla_\Sigma F)\cdot v_n\mathbf{n} + (\nabla F\cdot\mathbf{n})\mathbf{n}\cdot\mathbf{v_\Sigma}$$
$$+(\nabla F\cdot\mathbf{n})\mathbf{n}\cdot v_n\mathbf{n}\Big\}w_n\,\mathrm{d}\Sigma$$
$$+\int_\Sigma\Big\{F\Big[\operatorname{div}_\Sigma(\mathbf{v_\Sigma}+v_n\mathbf{n}) + D\mathbf{V}\mathbf{n}\cdot\mathbf{n}\Big]\Big\}w_n\,\mathrm{d}\Sigma.$$

Since $\operatorname{div}_\Sigma(v_n\mathbf{n}) = (\nabla_\Sigma v_n)\cdot\mathbf{n} + v_n\operatorname{div}_\Sigma\mathbf{n} = v_n\kappa$, one arrives at

$$\int_\Sigma[\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma$$
$$= \int_\Sigma\Big\{\nabla_\Sigma F\cdot\mathbf{v_\Sigma} + v_n\frac{\partial F}{\partial\mathbf{n}}$$
$$+F(\operatorname{div}_\Sigma\mathbf{v_\Sigma} + v_n\kappa + D\mathbf{V}\mathbf{n}\cdot\mathbf{n})\Big\}w_n\,\mathrm{d}\Sigma$$
$$= \int_\Sigma\Big\{\Big(\frac{\partial F}{\partial\mathbf{n}} + \kappa F\Big)v_n + F(\operatorname{div}_\Sigma\mathbf{v_\Sigma} + D\mathbf{V}\mathbf{n}\cdot\mathbf{n})$$
$$+\nabla_\Sigma F\cdot\mathbf{v_\Sigma}\Big\}w_n\,\mathrm{d}\Sigma$$
$$= \int_\Sigma\Big\{\Big(\frac{\partial F}{\partial\mathbf{n}} + \kappa F\Big)v_nw_n + FD\mathbf{V}\mathbf{n}\cdot\mathbf{n}w_n$$
$$+(\operatorname{div}_\Sigma(F\mathbf{v_\Sigma}))w_n\Big\}\,\mathrm{d}\Sigma. \tag{70}$$

Adding the vanishing term $(-\kappa Fw_n\mathbf{v_\Sigma}\cdot\mathbf{n})$ in the integral and applying the tangential Stoke's formula (18), we obtain

$$\int_\Sigma[\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma \tag{71}$$
$$= \int_\Sigma\Big\{\Big(\frac{\partial F}{\partial\mathbf{n}} + \kappa F\Big)v_nw_n + FD\mathbf{V}\mathbf{n}\cdot\mathbf{n}w_n$$
$$-\operatorname{div}_\Sigma(Fw_n\mathbf{v_\Sigma}) + (\operatorname{div}_\Sigma(F\mathbf{v_\Sigma}))w_n\Big\}\,\mathrm{d}\Sigma.$$

Applying the tangential divergence formula (17), we can express (71) as

$$\int_\Sigma[\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma$$
$$= \int_\Sigma\Big\{\Big(\frac{\partial F}{\partial\mathbf{n}} + \kappa F\Big)v_nw_n + FD\mathbf{V}\mathbf{n}\cdot\mathbf{n}w_n$$
$$-\nabla_\Sigma(Fw_n)\cdot\mathbf{v_\Sigma} - Fw_n\operatorname{div}_\Sigma\mathbf{v_\Sigma}\Big\}\,\mathrm{d}\Sigma$$
$$+\int_\Sigma\Big\{(\nabla_\Sigma F\cdot\mathbf{v_\Sigma})w_n + (F\operatorname{div}_\Sigma\mathbf{v_\Sigma})w_n\Big\}\,\mathrm{d}\Sigma.$$

Expanding the tangential gradient of Fw_n and simplifying the terms, we have

$$\int_\Sigma[\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma = \int_\Sigma\Big\{\Big(\frac{\partial F}{\partial\mathbf{n}} + \kappa F\Big)v_nw_n$$
$$+F(D\mathbf{V}\mathbf{n}\cdot\mathbf{n}w_n - \mathbf{v_\Sigma}\cdot\nabla_\Sigma w_n)\Big\}\,\mathrm{d}\Sigma. \tag{72}$$

In view of (63) and $D\mathbf{n} = D_\Sigma\mathbf{n}$, we obtain

$$D\mathbf{V}\mathbf{n}\cdot\mathbf{n}w_n = (D\mathbf{V})\mathbf{W}\cdot\mathbf{n} - \mathbf{w_\Sigma}\cdot(\nabla_\Sigma v_n - D_\Sigma\mathbf{n}\mathbf{v_\Sigma}), \tag{73}$$

and when we substitute this into (72) and rearrange the terms we get

$$\int_\Sigma[\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma = \int_\Sigma\Big\{\Big(\frac{\partial F}{\partial\mathbf{n}} + \kappa F\Big)v_nw_n$$
$$+F\Big((D_\Sigma\mathbf{n}\mathbf{v_\Sigma})\cdot\mathbf{w_\Sigma} - \mathbf{v_\Sigma}\cdot\nabla_\Sigma w_n - \mathbf{w_\Sigma}\cdot\nabla_\Sigma v_n\Big)$$
$$+F(D\mathbf{V})\mathbf{W}\cdot\mathbf{n}\Big\}\,\mathrm{d}\Sigma.$$

Using the identities in (65), this can be written as

$$\int_\Sigma[\operatorname{div}(F\mathbf{V})]\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma = \int_\Sigma\Big(\frac{\partial F}{\partial\mathbf{n}} + \kappa F\Big)v_nw_n\,\mathrm{d}\Sigma$$
$$-\int_\Sigma F\Big(\mathbf{v_\Sigma}\cdot(D_\Sigma\mathbf{n})\mathbf{w_\Sigma} + \mathbf{n}\cdot(D_\Sigma\mathbf{v})\mathbf{w_\Sigma}$$
$$+\mathbf{n}\cdot(D_\Sigma\mathbf{w})\mathbf{v_\Sigma}\Big)\,\mathrm{d}\Sigma$$
$$+\int_\Sigma F(D\mathbf{V})\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma.$$

Combining this with (82), we again obtain the same expression for the second-order Eulerian derivative of J, that is,

$$d^2J(\Omega;\mathbf{V},\mathbf{W}) = \frac{1}{2}\int_\Sigma F'_Wv_n\,\mathrm{d}\Sigma$$
$$+\frac{1}{2}\int_\Sigma\Big\{\Big(\frac{\partial F}{\partial\mathbf{n}} + \kappa F\Big)v_nw_n - F\Big(\mathbf{v_\Sigma}\cdot(D_\Sigma\mathbf{n})\mathbf{w_\Sigma}$$
$$+\mathbf{n}\cdot(D_\Sigma\mathbf{v})\mathbf{w_\Sigma} + \mathbf{n}\cdot(D_\Sigma\mathbf{w})\mathbf{v_\Sigma}\Big)\Big\}\,\mathrm{d}\Sigma$$
$$+\frac{1}{2}\int_\Sigma F(D\mathbf{V})\mathbf{W}\cdot\mathbf{n}\,\mathrm{d}\Sigma$$

D. The explicit form of $d^2J(\Omega;\mathbf{V},\mathbf{W})$

1) Computing $\int_\Sigma F'_Wv_n$: We turn to a discussion of the term $\int_\Sigma F'_Wv_n$. We consider (69) and write the integral

$\int_\Sigma F'_W v_n$ as follows:

$$\begin{aligned}\int_\Sigma F'_W v_n &= -2\int_\Sigma \frac{\partial u_D}{\partial \mathbf{n}}[\nabla u'_{D,W}\cdot \mathbf{n}\\ &\qquad +\nabla u_D\cdot \mathbf{N}'_W]v_n\,\mathrm{d}\Sigma\\ &+2\int_\Sigma \lambda(\kappa'_W u_N+\kappa u'_{N,W})v_n\,\mathrm{d}\Sigma\\ &-2\int_\Sigma \frac{\partial u_N}{\partial \tau}[\nabla u'_{N,W}\cdot\tau+\nabla u_N\cdot\tau'_W]v_n\,\mathrm{d}\Sigma\\ &=: M_1+M_2+M_3.\end{aligned}$$

First we examine M_1. Using (33), we write M_1 as

$$\begin{aligned}M_1 &= \int_\Sigma -2\frac{\partial u_D}{\partial \mathbf{n}}\left[\frac{\partial u'_{D,W}}{\partial \mathbf{n}}+\frac{\partial u_D}{\partial \mathbf{n}}\mathbf{n}\cdot[(D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n}\right.\\ &\quad \left.-(D\mathbf{W})^T\mathbf{n}-D\mathbf{n}\mathbf{W}]\right]v_n\,\mathrm{d}\Sigma\\ &= -2\int_\Sigma \frac{\partial u_D}{\partial \mathbf{n}}\left[\frac{\partial u'_{D,W}}{\partial \mathbf{n}}+\frac{\partial u_D}{\partial \mathbf{n}}(D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\right.\\ &\quad \left.-\frac{\partial u_D}{\partial \mathbf{n}}(D\mathbf{W}\mathbf{n}\cdot\mathbf{n})-\frac{\partial u_D}{\partial \mathbf{n}}\mathbf{n}\cdot D\mathbf{n}\mathbf{W}\right]v_n\,\mathrm{d}\Sigma.\end{aligned}$$

Because $\mathbf{n}^T D\mathbf{n}=0$ on Σ we further simplify M_1 as

$$M_1 = -2\int_\Sigma \frac{\partial u_D}{\partial \mathbf{n}}\frac{\partial u'_{D,W}}{\partial \mathbf{n}}v_n\,\mathrm{d}\Sigma. \tag{74}$$

We introduce the bijective and symmetric Steklov-Poincaré operator (Dirichlet-to-Neumann operator) S, defined by (cf. [34], [36])

$$Su^* = \frac{\partial w^*}{\partial \mathbf{n}} \tag{75}$$

where w^* solves the mixed boundary condition

$$\left\{\begin{array}{rcll} -\Delta w^* &=& 0 & \text{in } \Omega,\\ w^* &=& 0 & \text{on } \Gamma,\\ w^* &=& u^* & \text{on } \Sigma.\end{array}\right. \tag{76}$$

Hence, $Su'_{D,W}=\dfrac{\partial u'_{D,W}}{\partial \mathbf{n}}$, where $u'_{D,W}$ satisfies (50). Since $u'_{D,W}=-\dfrac{\partial u_D}{\partial \mathbf{n}}w_n$ on Σ one can rewrite M_1 as

$$\begin{aligned}M_1 &= -2\int_\Sigma (Su'_{D,W})\frac{\partial u_D}{\partial \mathbf{n}}v_n\,\mathrm{d}\Sigma\\ &= 2\int_\Sigma \left[S\left(-\frac{\partial u_D}{\partial \mathbf{n}}w_n\right)\right]\left[-\frac{\partial u_D}{\partial \mathbf{n}}v_n\right]\mathrm{d}\Sigma.\end{aligned} \tag{77}$$

Similarly, by introducing another Steklov-Poincaré R (Neumann-to-Dirichlet operator), defined by

$$R\left(\frac{\partial w^*}{\partial \mathbf{n}}\right)=u^* \tag{78}$$

where u^* satisfies

$$\left\{\begin{array}{rcll} -\Delta u^* &=& 0 & \text{in } \Omega,\\ u^* &=& 0 & \text{on } \Gamma,\\ \dfrac{\partial u^*}{\partial \mathbf{n}} &=& \dfrac{\partial w^*}{\partial \mathbf{n}} & \text{on } \Sigma,\end{array}\right. \tag{79}$$

we obtain

$$R\left(\frac{\partial u'_{N,W}}{\partial \mathbf{n}}\right)=u'_{N,W},$$

where $u'_{N,W}$ satisfies (52). Hence, we write M_2 as follows:

$$\begin{aligned}M_2 &= 2\int_\Sigma \lambda(\kappa'_W u_N v_n)\,\mathrm{d}\Sigma+2\int_\Sigma \lambda\kappa u'_{N,W}v_n\,\mathrm{d}\Sigma\\ &= 2\int_\Sigma \lambda\Big\{\mathrm{Tr}\Big[D\Big((D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n}-(D\mathbf{W})^T\mathbf{n}\Big)\\ &\qquad -D\mathbf{n}D\mathbf{W}\Big]-\nabla\kappa\cdot\mathbf{W}\Big\}u_N v_n\,\mathrm{d}\Sigma\\ &\quad +2\int_\Sigma \lambda\kappa R\Big[\mathrm{div}_\Sigma(w_n\nabla_\Sigma u_N)+w_n\kappa\lambda)\Big]v_n\,\mathrm{d}\Sigma.\end{aligned} \tag{80}$$

Finally, we simplify M_3 using R and (39):

$$\begin{aligned}M_3 &= -2\int_\Sigma \frac{\partial u_N}{\partial \tau}\left[\frac{\partial u'_{N,W}}{\partial \tau'_W}+\nabla u_N\cdot\tau'_W\right]v_n\,\mathrm{d}\Sigma\\ &= -2\int_\Sigma \frac{\partial u_N}{\partial \tau}\Big\{\nabla\Big[R\Big(\mathrm{div}_\Sigma(w_n\nabla_\Sigma u_N)\\ &\qquad +w_n\kappa\lambda\Big)\Big]\cdot\tau\Big\}v_n\\ &\quad -2\int_\Sigma \frac{\partial u_N}{\partial \tau}\Big\{\nabla u_N\cdot\Big[\Big((D\mathbf{W})^T\mathbf{n}\cdot\tau\Big)\mathbf{n}\\ &\qquad -(D\tau)\mathbf{W}\Big]\Big\}v_n\,\mathrm{d}\Sigma.\end{aligned} \tag{81}$$

Combining (74), (80), and (81) we obtain an explicit expression for $\int_\Sigma F'_W v_n$:

$$\begin{aligned}\int_\Sigma F'_W v_n &= 2\int_\Sigma \left[S\left(-\frac{\partial u_D}{\partial \mathbf{n}}w_n\right)\right]\left[-\frac{\partial u_D}{\partial \mathbf{n}}v_n\right]\mathrm{d}\Sigma\\ &+2\int_\Sigma \lambda\Big\{\mathrm{Tr}\Big[D\Big((D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n}-(D\mathbf{W})^T\mathbf{n}\Big)\\ &\qquad -D\mathbf{n}D\mathbf{W}\Big]-\nabla\kappa\cdot\mathbf{W}\Big\}u_N v_n\,\mathrm{d}\Sigma\\ &+2\int_\Sigma \lambda\kappa R\Big[\mathrm{div}_\Sigma(w_n\nabla_\Sigma u_N)+w_n\kappa\lambda\Big]v_n\,\mathrm{d}\Sigma\\ &-2\int_\Sigma \frac{\partial u_N}{\partial \tau}\Big\{\nabla\Big[R\Big(\mathrm{div}_\Sigma(w_n\nabla_\Sigma u_N)\\ &\qquad +w_n\kappa\lambda\Big)\Big]\cdot\tau\Big\}v_n\,\mathrm{d}\Sigma\\ &-2\int_\Sigma \frac{\partial u_N}{\partial \tau}\Big\{\nabla u_N\cdot\Big[\Big((D\mathbf{W})^T\mathbf{n}\cdot\tau\Big)\mathbf{n}\\ &\qquad -(D\tau)\mathbf{W}\Big]\Big\}v_n\,\mathrm{d}\Sigma.\end{aligned} \tag{82}$$

2) Analyzing $\int_\Sigma \frac{\partial F}{\partial \mathbf{n}}v_n w_n$: Inserting the definition of F (44), we obtain

$$\begin{aligned}\int_\Sigma \frac{\partial F}{\partial \mathbf{n}}v_n w_n &= \int_\Sigma \frac{\partial}{\partial \mathbf{n}}\left(\lambda^2-\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2\right)v_n w_n\,\mathrm{d}\Sigma\\ &\quad +2\int_\Sigma \frac{\partial}{\partial \mathbf{n}}(\lambda\kappa u_N)v_n w_n\,\mathrm{d}\Sigma\\ &\quad -\int_\Sigma \frac{\partial}{\partial \mathbf{n}}\left(\frac{\partial u_N}{\partial \tau}\right)^2 v_n w_n\,\mathrm{d}\Sigma\\ &=: N_1+N_2+N_3.\end{aligned} \tag{83}$$

At first, we write N_1 as

$$N_1 = \int_\Sigma -2\frac{\partial u_D}{\partial \mathbf{n}}\frac{\partial^2 u_D}{\partial \mathbf{n}^2} v_n w_n.$$

To simplify this we use the Laplace-Beltrami operator Δ_Σ (cf. [32]) defined by

$$\Delta_\Sigma u = \mathrm{div}_\Sigma(\nabla_\Sigma u),$$

which is related to the usual Laplace operator as

$$\Delta u = \Delta_\Sigma u + \kappa\frac{\partial u}{\partial \mathbf{n}} + \frac{\partial^2 u}{\partial \mathbf{n}^2}, \tag{84}$$

where κ represents the mean curvature of Σ. Note that the term $\dfrac{\partial^2 u}{\partial \mathbf{n}^2}$ can be written as $((\nabla^2 u)\mathbf{n})\cdot\mathbf{n}$, where $\nabla^2 u$ is the Hessian of u.

Using (84) we decompose Δu_D as

$$\Delta u_D = \Delta_\Sigma u_D + \kappa\frac{\partial u_D}{\partial \mathbf{n}} + \frac{\partial^2 u_D}{\partial \mathbf{n}^2}.$$

We know from (3) that the Laplacian of u_D vanishes. Since $u_D = 0$ on Σ, $\Delta_\Sigma u_D$ also vanishes. Hence we have $\dfrac{\partial^2 u_D}{\partial \mathbf{n}^2} = -\kappa\dfrac{\partial u_D}{\partial \mathbf{n}}$. Therefore,

$$N_1 = \int_\Sigma 2\kappa\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2 v_n w_n. \tag{85}$$

We write N_2 as

$$N_2 = 2\int_\Sigma \frac{\partial}{\partial \mathbf{n}}(\lambda\kappa u_N) v_n w_n \,\mathrm{d}\Sigma = 2\int_\Sigma (\lambda u_N \frac{\partial \kappa}{\partial \mathbf{n}} + \kappa\lambda^2). \tag{86}$$

Next, we observe that N_3 does not contribute at all because it can be written as

$$N_3 = -\int_\Sigma 2\frac{\partial u_N}{\partial \tau}\frac{\partial^2 u_N}{\partial \mathbf{n}\partial\tau} v_n w_n,$$

but

$$\frac{\partial^2 u_N}{\partial \mathbf{n}\partial \tau} = \frac{\partial}{\partial \tau}\left(\frac{\partial u_N}{\partial \mathbf{n}}\right) = \frac{\partial}{\partial\tau}(\lambda) = 0.$$

Combining (85) and (86) we obtain an expression for $\displaystyle\int_\Sigma \frac{\partial F}{\partial \mathbf{n}} v_n w_n$:

$$\int_\Sigma \frac{\partial F}{\partial \mathbf{n}} v_n w_n \,\mathrm{d}\Sigma = 2\int_\Sigma \kappa\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2 v_n w_n \,\mathrm{d}\Sigma + 2\int_\Sigma (\lambda u_N\frac{\partial\kappa}{\partial \mathbf{n}} + \kappa\lambda^2)\,\mathrm{d}\Sigma. \tag{87}$$

$$\int_\Sigma \frac{\partial F}{\partial \mathbf{n}} v_n w_n \,\mathrm{d}\Sigma = 2\int_\Sigma \kappa\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2 v_n w_n \,\mathrm{d}\Sigma + 2\int_\Sigma (\lambda u_N\frac{\partial\kappa}{\partial \mathbf{n}} + \kappa\lambda^2)\,\mathrm{d}\Sigma. \tag{88}$$

Finally, we insert (88) and (82) into (68) to obtain the explicit representation of the second-order Eulerian derivative of J associated with the exterior Bernoulli free boundary problem:

$$\begin{aligned}
d^2J(\Omega;\mathbf{V},\mathbf{W}) &= \int_\Sigma \left[S\left(-\frac{\partial u_D}{\partial \mathbf{n}}w_n\right)\right]\left[-\frac{\partial u_D}{\partial \mathbf{n}}v_n\right]\mathrm{d}\Sigma \\
&+ \int_\Sigma \lambda\Big\{\mathrm{Tr}\Big[D\Big((D\mathbf{W}\mathbf{n}\cdot\mathbf{n})\mathbf{n} - (D\mathbf{W})^T\mathbf{n}\Big) \\
&\qquad -D\mathbf{n}D\mathbf{W}\Big] - \nabla\kappa\cdot\mathbf{W}\Big\}u_N v_n \,\mathrm{d}\Sigma \\
&+ \int_\Sigma \lambda\kappa R\Big[\mathrm{div}_\Sigma(w_n\nabla_\Sigma u_N) + w_n\kappa\lambda\Big]v_n\,\mathrm{d}\Sigma \\
&- \int_\Sigma \frac{\partial u_N}{\partial\tau}\Big\{\nabla\Big[R\Big(\mathrm{div}_\Sigma(w_n\nabla_\Sigma u_N) \\
&\qquad + w_n\kappa\lambda\Big)\Big]\cdot\tau\Big\}v_n\,\mathrm{d}\Sigma \\
&- \int_\Sigma \frac{\partial u_N}{\partial\tau}\Big\{\nabla u_N\cdot\Big[\Big((D\mathbf{W})^T\mathbf{n}\cdot\tau\Big)\mathbf{n} \\
&\qquad -(D\tau)\mathbf{W}\Big]\Big\}v_n\,\mathrm{d}\Sigma \\
&+ \int_\Sigma \kappa\left(\frac{\partial u_D}{\partial \mathbf{n}}\right)^2 v_n w_n\,\mathrm{d}\Sigma + \int_\Sigma (\lambda u_N\frac{\partial\kappa}{\partial \mathbf{n}} + \kappa\lambda^2)\,\mathrm{d}\Sigma \\
&+ \frac{1}{2}\int_\Sigma \Big\{\Big[\lambda^2 - (\frac{\partial u_D}{\partial \mathbf{n}})^2 + 2\lambda\kappa u_N - (\frac{\partial u_N}{\partial\tau})^2\Big] \\
&\qquad \Big[\kappa v_n w_n - \Big(\mathbf{v_\Sigma}\cdot D_\Sigma\mathbf{n}\mathbf{w_\Sigma} + \mathbf{n}\cdot(D_\Sigma\mathbf{v})\mathbf{w_\Sigma} \\
&\qquad + \mathbf{n}\cdot(D_\Sigma\mathbf{w})\mathbf{v_\Sigma}\Big)\Big]\Big\}\,\mathrm{d}\Sigma \\
&+ \frac{1}{2}\int_\Sigma \Big\{\Big[\lambda^2 - (\frac{\partial u_D}{\partial \mathbf{n}})^2 + 2\lambda\kappa u_N - (\frac{\partial u_N}{\partial\tau})^2\Big] \\
&\qquad [(D\mathbf{V})\mathbf{W}\cdot\mathbf{n}]\Big\}\,\mathrm{d}\Sigma.
\end{aligned} \tag{89}$$

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