

Electrostatic Force Computation Using Shape Calculus

Master Thesis Project

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Abstract

In Electrostatics, it is often of interest to compute local/global forces on a body in electrostatic equilibrium. The classical formula for computing this force is a surface/volume integral, obtained using the Maxwell Stress Tensor. In the surface integral form it has some undesirable properties, affecting the accuracy when used with Boundary Element Methods. In this work, we explore a new approach for calculating the force using shape calculus, in an effort to find a stable formula on the boundary which can be used with BEM. The properties of this new formula are discussed using numerical experiments.

1 Introduction

In Electrodynamics, it is of interest to compute the electromagnetic forces. The forces can be written in a compact way by introduction of the Maxwell stress tensor. For a linear medium, the Maxwell stress tensor is defined as follows [2, Ch. 8, eq. 8.17]:

$$T_{ij} := \epsilon_0(E_i E_j - \frac{1}{2}\delta_{ij}E^2) + \frac{1}{\mu_0}(B_i B_j - \frac{1}{2}\delta_{ij}B^2), \quad i, j \in \{1, 2, 3\}, \quad (1.1)$$

\mathbf{B} and \mathbf{E} are the magnetic and electric fields respectively. Using the Maxwell stress tensor, the force density \mathbf{f} can be written as:

$$\mathbf{f} = \nabla \cdot T - \epsilon_0 \mu_0 \frac{\partial \mathbf{S}}{\partial t}, \quad (1.2)$$

Where \mathbf{S} is the Poynting vector given as:

$$\mathbf{S} := \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B}. \quad (1.3)$$

In this work, we deal with electrostatics only where the magnetic field \mathbf{B} and all time derivatives are equal to zero. The formulas reduce to:

$$T_{ij} = \epsilon_0(E_i E_j - \frac{1}{2}\delta_{ij}E^2), \quad (1.4)$$

$$\mathbf{f} = \nabla \cdot T. \quad (1.5)$$

The total electrostatic force on the charges contained within a volume Ω can be found by integrating the force density over the volume:

$$\mathbf{F} = \int_{\Omega} \mathbf{f} \, dx = \int_{\Omega} \nabla \cdot T \, dx. \quad (1.6)$$

Using Divergence theorem we find an equivalent surface integral form for the force:

$$\mathbf{F} = \int_{\partial\Omega} T \cdot \mathbf{n} \, dS. \quad (1.7)$$

We know that $\nabla u = -\mathbf{E}$ where u is the electrostatic potential. Assuming $\epsilon_0 = 1$:

$$\mathbf{F} = \int_{\partial\Omega} \nabla u \cdot \mathbf{n} \, \nabla u \, dS - \frac{1}{2} \int_{\partial\Omega} \|\nabla u\|^2 \mathbf{n} \, dS. \quad (1.8)$$

For simplicity, we talk about the case of a perfect conductor where \mathbf{E} is in the normal direction at the surface:

$$\nabla u = (\nabla u \cdot \mathbf{n}) \mathbf{n}. \quad (1.9)$$

The formula for the total force reduces to:

$$\mathbf{F} = \frac{1}{2} \int_{\partial\Omega} (\nabla u \cdot \mathbf{n})^2 \mathbf{n} \, dS. \quad (1.10)$$

We observe that $\nabla u \cdot \mathbf{n}$ is the Neumann Trace which is in the space $H^{-\frac{1}{2}}(\partial\Omega)$ but it must belong to $L^2(\partial\Omega)$ for the above formula to be well defined. Since $L^2(\partial\Omega) \subset H^{-\frac{1}{2}}(\partial\Omega)$, the integral for total force is unbounded on the energy trace space $H^{-\frac{1}{2}}(\partial\Omega)$, as a consequence of which the superconvergence of the Galerkin approximation for total force is not guaranteed anymore [4, Section 5.6]. For this reason the force formula suffers numerically, even in some cases when the Neumann trace is in $L^2(\partial\Omega)$. This is the motivation for this work where we try to find a numerically stable formula using shape calculus. The idea is that the shape gradient of energy functional gives us the force in some sense.

2 Energy shape gradient using BEM

The setting for this work is Electrostatics with a Dirichlet boundary value problem (BVP) posed on an open bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ with a piecewise smooth boundary $\partial\Omega$. We are interested in computing the electrostatic force on this domain. The electrostatic potential u solves :

$$\Delta u = 0 \quad \text{in } \Omega, \quad u = g \quad \text{on } \Gamma := \partial\Omega.$$

We assume that the material is a linear and homogeneous dielectric. We solve the Dirichlet BVP with direct first kind Boundary Element Method (BEM) using piecewise constant trial and test functions.

Note: For derivation of the shape gradient formula, g is required to be defined in the volume, not just the boundary. This is required for the Dirichlet BVP to be well defined when the domain is perturbed.

2.1 Direct first kind BIE

In the direct first kind BIE for Dirichlet BVP, we seek $\Psi \in H^{-\frac{1}{2}}(\Gamma)$ such that:

$$a_V(\Psi, \Phi) = \frac{1}{2}l(\Phi) + a_K(\Phi) \quad \forall \Phi \in H^{-\frac{1}{2}}(\Gamma). \quad (2.1)$$

The equation above is the variational formulation for the direct first kind BIE, where a_V and a_K are the variational forms for the Single Layer and Double Layer boundary integral operators (BIO) respectively, and l is the variational form for the identity operator. The terms in the formulation are defined as:

$$a_V(\Psi, \Phi) := \int_{\Gamma} \int_{\Gamma} G(x, y) \Psi(y) \Phi(x) d\Gamma(x) d\Gamma(y), \quad (2.2)$$

$$a_K(\Phi) := \int_{\Gamma} \int_{\Gamma} \nabla_y G(x, y) \cdot \mathbf{n}(y) g(y) \Phi(x) d\Gamma(x) d\Gamma(y), \quad (2.3)$$

$$l(\Phi) := \int_{\Gamma} g(x) \Phi(x) d\Gamma(\hat{x}). \quad (2.4)$$

$G(x, y)$ is the fundamental solution for the Laplace operator, g is the Dirichlet data and $\Psi := \nabla u \cdot \mathbf{n}$ is the Neumann trace of the potential u . We use the following energy functional:

$$\begin{aligned} &= \frac{1}{2} \int_{\Omega} |\nabla u|^2 dx = \frac{1}{2} \int_{\Gamma} \Psi(x) g(x) d\Gamma \quad \text{for } \Delta u = 0, \\ J(\Psi) &:= \frac{1}{2} \int_{\Gamma} \Psi(x) g(x) d\Gamma. \end{aligned} \quad (2.5)$$

Note: The electrostatic field energy is given as

$$\frac{\epsilon_0}{2} \int_{\mathbb{R}^3} |\nabla u|^2 dx, \quad (2.6)$$

which involves the integral over the whole space. The chosen energy functional in eq. (2.5) is artificial as it represents the true electrostatic field energy only when the electric field \mathbf{E} is zero in Ω' (complement of Ω) or in other words, when Ω' is a conductor and Ω is a cavity in the conductor.

2.2 Shape Calculus

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ be an open bounded Lipschitz domain with a piecewise smooth boundary $\partial\Omega$ and let $J(\Omega) \in \mathbb{R}$ be a real-valued quantity associated to it. One is often interested in quantifying the shape sensitivity of J i.e. how $J(\Omega)$ changes with respect to slight changes in Ω [8]. In this work, we use the perturbation approach to model these changes in Ω . We define a perturbation map T_t :

$$\begin{aligned} T_t &: \mathbb{R}^d \rightarrow \mathbb{R}^d, \\ T_t(x) &:= x + t \nu(x), \quad \nu(x) \in C^1(\mathbb{R}^d; \mathbb{R}^d), \quad t \in \mathbb{R}, \end{aligned} \quad (2.7)$$

where ν is a velocity field. Assuming $\|\nu\|_{C^1}$ is bounded, the perturbation map above can be proved to be a diffeomorphism for small t . It is therefore natural to consider $J(\Omega)$ as the realization of a shape functional [8]:

$$J : U_{adm} \rightarrow \mathbb{R},$$

where U is the set of admissible domains, defined as the set of perturbations of a reference domain Ω_0 :

$$U_{adm} := \{T_t(\Omega_0) : |t| < 1, \|\nu\|_{C^1} < 1\}. \quad (2.8)$$

The domains in this set are parametrized by the scalar t . The shape gradient at Ω can be defined as the following directional Eulerian derivative:

$$\frac{dJ}{d\Omega}(\Omega; \nu) = \lim_{t \rightarrow 0} \frac{J(T_t(\Omega)) - J(\Omega)}{t}. \quad (2.9)$$

It is desirable that (2.9) exists for all ν . It is then natural to say that J is shape differentiable if the mapping

$$\frac{dJ}{d\Omega}(\Omega; \cdot) : C^1(\mathbb{R}^d; \mathbb{R}^d) \rightarrow \mathbb{R}, \quad \nu \mapsto \frac{dJ}{d\Omega}(\Omega; \nu), \quad (2.10)$$

is linear and bounded on $C^1(\mathbb{R}^d; \mathbb{R}^d)$. In literature, this mapping is called shape gradient of J at Ω [1, Ch. 9, Def. 2.2].

Remark 1. *In literature, the perturbations defined in eq. (2.7) are called perturbations of the identity. This approach is less general than the velocity method but leads to the same first order shape calculus [1, Ch. 9, Thm 3.2].*

Remark 2. *The Hadamard structure theorem [1, Ch. 9, Thm 3.6] states that if $\partial\Omega$ is smooth, $\frac{dJ}{d\Omega}(\Omega; \nu)$ admits a representative $f(\Omega)$ in the space of distributions $\mathcal{D}^k(\partial\Omega)$ such that*

$$\frac{dJ}{d\Omega}(\Omega; \nu) = \langle f(\Omega), \nu \cdot n|_{\partial\Omega} \rangle_{\mathcal{D}^k(\partial\Omega)}. \quad (2.11)$$

Eq. (2.11) states that only the normal component of the velocity field on the boundary changes the value of the shape functional, which makes sense as only the normal component of the velocity field changes the shape.

2.3 Shape gradient with BIE constraint

Now, we want to find the shape gradient of the energy functional using the definition from eq. (2.9). But, the energy functional in eq. (2.5) depends not only on the domain Ω , but also on the Neumann Trace Ψ which in turn depends on the domain Ω :

$$J = J(\Omega, \Psi(\Omega)) = \mathcal{J}(\Omega). \quad (2.12)$$

So we have to compute the shape gradient of the energy functional, constrained by the direct first kind BIE. To evaluate the shape gradient in this case, we use the Lagrangian approach. We think of the BIE being defined on the set of admissible domains which is parametrized by the scalar t . So we admit the shape parameter 't' into the BIE:

$$\implies \quad a_V(\Psi, \Phi) \rightarrow a_V(t; \Psi, \Phi), \quad a_K(\Phi) \rightarrow a_K(t; \Phi), \quad l(\Phi) \rightarrow l(t; \Phi), \quad J(\Psi) \rightarrow J(t; \Psi).$$

The direct first kind BIE on the boundary $\Gamma_t := T_t(\Gamma_0)$ is given as:

$$\Psi_t \in H^{-\frac{1}{2}}(\Gamma_t) : \quad a_V(t; \Psi_t, \Phi) = a_K(t; \Phi) + \frac{1}{2}l(t; \Phi), \quad \forall \Phi \in H^{-\frac{1}{2}}(\Gamma_t). \quad (2.13)$$

Ψ_t is the Neumann Trace solution of the BIE posed on the boundary Γ_t . Integrals appearing in the BIE can be transformed to the reference boundary Γ_0 , using the perturbation map (2.7) and the following transformation rule [1, Ch. 9, Sec. 4.2, eq. 4.9]:

$$\int_{\Gamma_t} f(x) d\Gamma_t(x) = \int_{\Gamma_0} f(T_t(\hat{x})) \omega_t(\hat{x}) d\Gamma_0(\hat{x}), \quad \omega_t(\hat{x}) = |M(DT_t)(\hat{x}) \hat{\mathbf{n}}(\hat{x})|, \quad (2.14)$$

where $M(A)$ is the cofactor matrix of A and $\hat{\mathbf{n}}$ is the unit normal field on Γ_0 . DT_t is the Jacobian matrix for the transformation T_t , given as $DT_t(i, j) = \frac{\partial T_t(i)}{\partial x_j}$. Using the identity above, the integrals in the BIE can be transformed to the reference boundary Γ_0 :

$$J(t; \Psi) = \frac{1}{2} \int_{\Gamma_0} \Psi(T_t(\hat{x})) g(T_t(\hat{x})) \omega_t(\hat{x}) d\Gamma_0(\hat{x}), \quad (2.15)$$

$$a_V(t; \Psi, \Phi) = \int_{\Gamma_0} \int_{\Gamma_0} G(T_t(\hat{x}), T_t(\hat{y})) \Psi(T_t(\hat{y})) \Phi(T_t(\hat{x})) \omega_t(\hat{x}) \omega_t(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \quad (2.16)$$

The unit normal transforms as follows [1, Ch. 9, Thm. 4.4]:

$$\mathbf{n}(x) = \frac{M(DT_t)(\hat{x}) \hat{\mathbf{n}}(\hat{x})}{|M(DT_t)(\hat{x}) \hat{\mathbf{n}}(\hat{x})|} = \frac{M(DT_t)(\hat{x}) \hat{\mathbf{n}}(\hat{x})}{\omega_t(\hat{x})}, \quad (2.17)$$

where \mathbf{n} and $\hat{\mathbf{n}}$ are unit normal fields on Γ_t and Γ_0 respectively. The remaining terms in BIE transform as:

$$a_K(t; \Phi) = \int_{\Gamma_0} \int_{\Gamma_0} \{ \nabla_y G(T_t(\hat{x}), T_t(\hat{y})) \cdot M(DT_t)(\hat{y}) \hat{\mathbf{n}}(\hat{y}) \} g(T_t(\hat{y})) \Phi(T_t(\hat{x})) \omega_t(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \quad (2.18)$$

$$l(t; \Phi) = \int_{\Gamma_0} g(T_t(\hat{x})) \Phi(T_t(\hat{x})) \omega_t(\hat{x}) d\Gamma_0(\hat{x}). \quad (2.19)$$

2.3.1 Pullback Approach

In the integrals transformed back to the reference boundary, both Φ and Ψ belong to the space $H^{-\frac{1}{2}}(\Gamma_t)$, so we define the following pullback:

$$\gamma_t^* \Phi(\hat{x}) := \Phi(T_t(\hat{x})) = \hat{\Phi}(t; \hat{x}), \quad \Phi \in H^{-\frac{1}{2}}(\Gamma_t), \quad \hat{\Phi} \in H^{-\frac{1}{2}}(\Gamma_0). \quad (2.20)$$

We can find a function $\hat{\Phi} \in H^{-\frac{1}{2}}(\Gamma_0)$ for any $\Phi \in H^{-\frac{1}{2}}(\Gamma_t)$. The idea is to get rid of the 't' dependence of spaces using the pullback. Using that we get:

$$\begin{aligned} J(t; \Psi) &= \tilde{J}(t; \hat{\Psi}) &= \frac{1}{2} \int_{\Gamma_0} \hat{\Psi}(t; \hat{x}) g(T_t(\hat{x})) \omega_t(\hat{x}) d\Gamma_0(\hat{x}), \\ a_V(t; \Psi, \Phi) &= \tilde{a}_V(t; \hat{\Psi}, \hat{\Phi}) &= \int_{\Gamma_0} \int_{\Gamma_0} G(T_t(\hat{x}), T_t(\hat{y})) \hat{\Psi}(t; \hat{y}) \hat{\Phi}(\hat{x}) \omega_t(\hat{x}) \omega_t(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \\ a_K(t; \Phi) &= \tilde{a}_K(\hat{\Phi}) &= \int_{\Gamma_0} \int_{\Gamma_0} (\nabla_y G(T_t(\hat{x}), T_t(\hat{y})) \cdot M(DT_t)(\hat{y}) \hat{\mathbf{n}}(\hat{y})) g(T_t(\hat{y})) \hat{\Phi}(\hat{x}) \omega_t(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \\ l(t; \Phi) &= \tilde{l}(t; \hat{\Phi}) &= \int_{\Gamma_0} g(T_t(\hat{x})) \hat{\Phi}(\hat{x}) \omega_t(\hat{x}) d\Gamma_0(\hat{x}). \end{aligned}$$

Note: We don't use a pullback for the function g as it is a function defined in the volume, independent of any domain transformations. Using the pullback on Φ , we write $\hat{\Phi}(\hat{x})$ instead of $\hat{\Phi}(t; \hat{x})$ because Φ is a test function in the formulation and does not depend on t . Using all $\Phi \in H^{-\frac{1}{2}}(\Gamma_t)$ means using all $\hat{\Phi} \in H^{-\frac{1}{2}}(\Gamma_0)$.

2.3.2 Lagrangian Approach

Using the pullback defined in the previous section, we get rid of the 't' dependence of spaces and can finally use the Lagrangian approach. The Lagrangian is defined using the tilde quantities as:

$$L(t; \hat{\Psi}, \hat{\Phi}) := \tilde{J}(t; \hat{\Psi}) + \tilde{a}_V(t; \hat{\Psi}, \hat{\Phi}) - \frac{1}{2} \tilde{l}(t; \hat{\Phi}) - \tilde{a}_K(t; \hat{\Phi}), \quad \hat{\Psi} \in H^{-\frac{1}{2}}(\Gamma_0), \quad \hat{\Phi} \in H^{-\frac{1}{2}}(\Gamma_0). \quad (2.21)$$

We plug in $\hat{\Psi}_t$ in place of $\hat{\Psi}$ in eq. (2.21), such that $\hat{\Psi}_t$ is the pullback for the state solution on Γ_t :

$$\begin{aligned} \hat{\Psi}_t &= \hat{\Psi}_t(t; \hat{x}) = \Psi_t(T_t(\hat{x})) : \quad a_V(t; \Psi_t, \Phi) = \frac{1}{2}l(t; \Phi) + a_K(t; \Phi) \quad \forall \Phi \in H^{-\frac{1}{2}}(\Gamma_t). \\ \implies L(t; \hat{\Psi}_t, \hat{\Phi}) &= J(t; \hat{\Psi}_t) = \mathcal{J}(t) \quad \forall \hat{\Phi} \in H^{-\frac{1}{2}}(\Gamma_0). \end{aligned} \quad (2.22)$$

Since t is the parameter representing some domain from the space of admissible domains, the equation above can be equivalently written as:

$$L(\Omega; \hat{\Psi}_\Omega, \hat{\Phi}) = J(\Omega; \hat{\Psi}_\Omega) = \mathcal{J}(\Omega). \quad (2.23)$$

Differentiating the above equation using chain rule we get:

$$\frac{d\mathcal{J}}{d\Omega}(\Omega; \nu)|_{\Omega=\Omega_0} = \frac{\partial L}{\partial \Omega}(\Omega; \hat{\Psi}_\Omega, \hat{\Phi})|_{\Omega=\Omega_0} + \frac{\partial L}{\partial \hat{\Psi}}(\Omega, \hat{\Psi}_\Omega, \hat{\Phi}; \frac{d\hat{\Psi}_\Omega}{d\Omega}(\Omega; \nu))|_{\Omega=\Omega_0}. \quad (2.24)$$

Shape gradient of the state solution highlighted above is difficult to compute. In the Lagrangian approach, we fix $\hat{\Phi} = p$ such that the second term is always zero:

$$\frac{\partial L}{\partial \hat{\Psi}}(\Omega, \hat{\Psi}_\Omega, p; v)|_{\Omega=\Omega_0} = 0 \quad \forall v \in H^{-\frac{1}{2}}(\Gamma_0). \quad (2.25)$$

Using the definition of the Lagrangian in (2.21), the LHS in equation above can be written as:

$$\begin{aligned} \frac{\partial L}{\partial \hat{\Psi}}(\Omega, \hat{\Psi}_\Omega, p; v)|_{\Omega=\Omega_0} &= \frac{\partial \tilde{J}}{\partial \hat{\Psi}}(\Omega, \hat{\Psi}_\Omega; v)|_{\Omega=\Omega_0} + \frac{\partial \tilde{a}_V}{\partial \hat{\Psi}}(\Omega, \hat{\Psi}_\Omega, p; v)|_{\Omega=\Omega_0} \\ &\equiv \frac{\partial \tilde{J}}{\partial \hat{\Psi}}(t, \hat{\Psi}_t; v)|_{t=0} + \frac{\partial \tilde{a}_V}{\partial \hat{\Psi}}(t, \hat{\Psi}_t, p; v)|_{t=0}. \end{aligned} \quad (2.26)$$

In the last step, we replace Ω by the scalar t which parametrizes the domain. Since both \tilde{a}_V and \tilde{J} are linear in $\hat{\Psi}$, we get:

$$\tilde{J}(t; v)|_{t=0} + \tilde{a}_V(t; v, p)|_{t=0} = 0. \quad (2.27)$$

Simplifying the above expression we get the adjoint equation:

$$p \in H^{-\frac{1}{2}}(\Gamma_0) : \quad a_V(p, v) = -J(v) \quad \forall v \in H^{-\frac{1}{2}}(\Gamma_0). \quad (2.28)$$

p is called the adjoint solution using which, the shape gradient we require is given as:

$$\frac{d\mathcal{J}}{d\Omega}(\Omega; \nu)|_{\Omega=\Omega_0} = \frac{\partial L}{\partial \Omega}(\Omega, \hat{\Psi}_\Omega, p)|_{\Omega=\Omega_0} \equiv \frac{\partial L}{\partial t}(t, \hat{\Psi}_t, p)|_{t=0}. \quad (2.29)$$

In the previous equation, we again use t and Ω interchangeably. To find the partial derivative with respect to t (at $t = 0$), we expand the t dependent terms using Taylor expansion and collect the terms linear in t .

Note: Since the derivative is partial with respect to t , we ignore the dependence of $\hat{\Psi}_t$ on t .

Taylor expansions and identities used to find the partial derivatives are summarized next. Using the perturbation map from eq. (2.7) we know:

$$DT_t = I + t D\nu = I + t \nabla \nu^T, \quad (2.30)$$

$$\det(DT_t) = 1 + t \nabla \cdot \nu + O(t^2). \quad (2.31)$$

We know that for any invertible matrix K [10, Sec. 2.2]:

$$(K^{-1})' = -K^{-1}K'K^{-1}. \quad (2.32)$$

Using the identities given above we find the Taylor expansion of DT_t^{-1} about $t = 0$. First we calculate its derivative:

$$\frac{d(DT_t^{-1})}{dt}|_{t=0} = -DT_t^{-1} \frac{d(DT_t)}{dt} DT_t^{-1}|_{t=0} = -I \nabla \nu^T I = -\nabla \nu^T. \quad (2.33)$$

The Taylor expansion is given as:

$$DT_t^{-1} = I - t \nabla \nu^T + O(t^2). \quad (2.34)$$

Using the Taylor expansion above, we get the expansion for the cofactor matrix of DT_t :

$$M(DT_t) = J_t DT_t^{-T} = (1 + t \nabla \cdot \nu + O(t^2))(I - t \nabla \nu^T + O(t^2))^T, \quad J_t := \det(DT_t) \quad (2.35)$$

$$= I + tA + O(t^2), \quad A = \nabla \cdot \nu I - \nabla \nu. \quad (2.36)$$

Using the Taylor expansion for the cofactor matrix we get the Taylor expansion for the metric of transformation ω_t :

$$\omega_t = |M(DT_t)n| = |n + tA n + O(t^2)| \quad (2.37)$$

$$= 1 + t n \cdot A n + O(t^2), \quad |n| = 1. \quad (2.38)$$

We also know

$$f \circ T_t = f + t \nabla f \cdot \nu + O(t^2). \quad (2.39)$$

$$G(T_t(\hat{x}), T_t(\hat{y})) = G(\hat{x}, \hat{y}) + t (\nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y}) + \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x})) + O(t^2). \quad (2.40)$$

The J term, using eq. (2.39) and (2.38)

$$\begin{aligned} &= \frac{1}{2} \int_{\Gamma_0} \hat{\Psi}_t(t, \hat{x}) g(T_t(\hat{x})) \omega_t(\hat{x}) d\Gamma_0(\hat{x}) \\ &= \frac{1}{2} \int_{\Gamma_0} \hat{\Psi}_t(t, \hat{x}) (g(\hat{x}) + t \nabla g(\hat{x}) \cdot \nu(\hat{x}) + O(t^2)) (1 + t \hat{\mathbf{n}}(\hat{x}) \cdot A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) + O(t^2)) d\Gamma_0(\hat{x}). \end{aligned}$$

Collecting the terms linear in t, the partial derivative for the J term at t = 0

$$= \frac{1}{2} \int_{\Gamma_0} \Psi_0(\hat{x}) (g(\hat{x}) \hat{\mathbf{n}}(\hat{x}) \cdot A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) + \nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}), \quad (2.41)$$

where Ψ_0 solves the state problem on Γ_0 . The a_V term, using eq. (2.40) and (2.38)

$$\begin{aligned} &= \int_{\Gamma_0} \int_{\Gamma_0} \hat{\Psi}_t(t, \hat{y}) (G(\hat{x}, \hat{y}) + t (\nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y})) + O(t^2)) \\ &\quad (1 + t \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) + O(t^2)) (1 + t \hat{\mathbf{n}}(\hat{y})^T A(\hat{y}) \hat{\mathbf{n}}(\hat{y}) + O(t^2)) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \end{aligned} \quad (2.42)$$

and the partial derivative at t = 0 is given as

$$\begin{aligned} &= \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \{ \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y}) \\ &\quad + G(\hat{x}, \hat{y}) (\hat{\mathbf{n}}(\hat{y})^T A(\hat{y}) \hat{\mathbf{n}}(\hat{y}) + \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x})) \} p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \end{aligned} \quad (2.43)$$

For treating the a_K term, the following Taylor expansion is used:

$$\nabla_y G(T_t(\hat{x}), T_t(\hat{y})) = \nabla_y G(\hat{x}, \hat{y}) + t \kappa(\hat{x}, \hat{y}) + O(t^2), \quad (2.44)$$

$$\kappa(\hat{x}, \hat{y}) := \frac{d(\nabla_y G(T_t(\hat{x}), T_t(\hat{y})))}{dt} \Big|_{t=0}. \quad (2.45)$$

Plugging in the above expansion and using eq. (2.38), (2.39) and (2.36), we get:

$$\begin{aligned} &= \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) (\nabla_y G(\hat{x}, \hat{y}) + t \kappa(\hat{x}, \hat{y}) + O(t^2)) \cdot (\hat{\mathbf{n}}(\hat{y}) + t A(\hat{y}) \hat{\mathbf{n}}(\hat{y}) + O(t^2)) \\ &\quad (g(\hat{y}) + t \nabla g(\hat{y}) \cdot \nu(\hat{y}) + O(t^2)) (1 + t \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) + O(t^2)) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \end{aligned} \quad (2.46)$$

and the partial derivative at $t = 0$ is given as

$$= \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) \kappa(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) + g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (A(\hat{y}) \hat{\mathbf{n}}(\hat{y})) + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) (\nabla g(\hat{y}) \cdot \nu(\hat{y})) \\ + g(\hat{y}) (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \quad (2.47)$$

The 1 term, using eq. (2.39) and (2.38)

$$= \int_{\Gamma_0} p(\hat{x}) (g(\hat{x}) + t \nabla g(\hat{x}) \cdot \nu(\hat{x}) + O(t^2)) (1 + t \hat{\mathbf{n}}(\hat{x}) \cdot A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) + O(t^2)) d\Gamma_0(\hat{x}), \quad (2.48)$$

and the partial derivative at $t = 0$ is given as

$$= \int_{\Gamma_0} p(\hat{x}) (g(\hat{x}) \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) + \nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}). \quad (2.49)$$

We add up the individual terms to get the final shape gradient:

$$= \frac{1}{2} \int_{\Gamma_0} \Psi_0(\hat{x}) (g(\hat{x}) \hat{\mathbf{n}}(\hat{x}) \cdot A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) + \nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\ + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \{ \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y}) \\ + G(\hat{x}, \hat{y}) (\hat{\mathbf{n}}(\hat{y})^T A(\hat{y}) \hat{\mathbf{n}}(\hat{y}) + \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x})) \} p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) \kappa(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) + g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (A(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\ + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) (\nabla g(\hat{y}) \cdot \nu(\hat{y})) + g(\hat{y}) (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) (g(\hat{x}) \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) + \nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}).$$

The terms highlighted in the above equation can be rearranged to give

$$= \frac{1}{2} \int_{\Gamma_0} \Psi_0(\hat{x}) g(\hat{x}) \hat{\mathbf{n}}(\hat{x}) \cdot A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) d\Gamma_0(\hat{x}) \\ + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) G(\hat{x}, \hat{y}) (\hat{\mathbf{n}}(\hat{y})^T A(\hat{y}) \hat{\mathbf{n}}(\hat{y})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) G(\hat{x}, \hat{y}) (\hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) g(\hat{x}) \hat{\mathbf{n}}(\hat{x})^T A(\hat{x}) \hat{\mathbf{n}}(\hat{x}) d\Gamma_0(\hat{x}) \\ = a_V(p, f1) + J(f1) + a_V(\Psi_0, f2) - a_K(f2) - \frac{1}{2} l(f2), \\ f1(x) = \Psi_0(x) \hat{\mathbf{n}}(x)^T A(x) \hat{\mathbf{n}}(x), \quad f2(x) = p(x) \hat{\mathbf{n}}(x)^T A(x) \hat{\mathbf{n}}(x).$$

Using the state and the adjoint equation on the boundary Γ_0 , the terms highlighted above give zero (assuming $f1, f2 \in H^{-\frac{1}{2}}(\Gamma_0)$), using which get the shape gradient formula.

Theorem 2.1. *The shape gradient for the energy functional from eq. (2.5), constrained by the direct first kind BIE for Dirichlet BVP is given as:*

$$\begin{aligned}
\frac{d\mathcal{J}}{d\Omega}(\Omega; \nu)|_{\Omega=\Omega_0} &= \frac{1}{2} \int_{\Gamma_0} \Psi_0(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
&+ \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \{ \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y}) \} p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&- \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) \kappa(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) + g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (A(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\
&+ (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) (\nabla g(\hat{y}) \cdot \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&- \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x})
\end{aligned} \tag{2.50}$$

2.3.3 Modified Pullback

In this subsection, we do the pullback approach with a modified pullback defined as:

$$\gamma_t^* \Psi(\hat{x}) := \Psi(T_t(\hat{x})) \omega_t(\hat{x}) = \hat{\Psi}(t; \hat{x}). \tag{2.51}$$

The idea is again to get rid of 't' dependence of spaces but here we also include the metric factor ω in the pullback to simplify things. Using this pullback on the BIE integrals transformed back to the reference boundary (eq. (2.15) to (2.19)), we get slightly different tilde quantities:

$$\begin{aligned}
J(t; \Psi) = \tilde{J}(t; \hat{\Psi}) &= \frac{1}{2} \int_{\Gamma_0} \hat{\Psi}(t; \hat{x}) g(T_t(\hat{x})) d\Gamma_0(\hat{x}), \\
a_V(t; \Psi, \Phi) = \tilde{a}_V(t; \hat{\Psi}, \hat{\Phi}) &= \int_{\Gamma_0} \int_{\Gamma_0} G(T_t(\hat{x}), T_t(\hat{y})) \hat{\Psi}(t; \hat{y}) \hat{\Phi}(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \\
a_K(t; \Phi) = \tilde{a}_K(t; \hat{\Phi}) &= \int_{\Gamma_0} \int_{\Gamma_0} (\nabla_y G(T_t(\hat{x}), T_t(\hat{y})) \cdot M(DT_t)(\hat{y}) \hat{\mathbf{n}}(\hat{y})) g(T_t(\hat{y})) \hat{\Phi}(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \\
l(t; \Phi) = \tilde{l}(t; \hat{\Phi}) &= \int_{\Gamma_0} g(T_t(\hat{x})) \hat{\Phi}(\hat{x}) d\Gamma_0(\hat{x}).
\end{aligned}$$

Using the Lagrangian approach described in section 2.3.2 and the Taylor expansions, we can find the shape gradient for this modified pullback approach. The adjoint equation and its solution remain unchanged as the new \tilde{a}_V and \tilde{J} are still linear in $\hat{\Psi}$. To find the shape gradient we again evaluate the partial derivatives with respect to t . For the J term, using eq. (2.39):

$$\begin{aligned}
&= \frac{1}{2} \int_{\Gamma_0} \hat{\Psi}_t(t, \hat{x}) g(T_t(\hat{x})) d\Gamma_0(\hat{x}) \\
&= \frac{1}{2} \int_{\Gamma_0} \hat{\Psi}_t(t, \hat{x}) (g(\hat{x}) + t \nabla g(\hat{x}) \cdot \nu(\hat{x}) + O(t^2)) d\Gamma_0(\hat{x}).
\end{aligned}$$

The partial derivative for the J term, at $t = 0$:

$$= \frac{1}{2} \int_{\Gamma_0} \Psi_0(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}). \tag{2.52}$$

Ψ_0 solves the state problem on Γ_0 . For the a_V term using eq. (2.40):

$$= \int_{\Gamma_0} \int_{\Gamma_0} (G(\hat{x}, \hat{y}) + t (\nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y})) + O(t^2)) \hat{\Psi}_t(t, \hat{y}) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \tag{2.53}$$

and the partial derivative at $t = 0$ is given as:

$$= \int_{\Gamma_0} \int_{\Gamma_0} (\nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y})) \Psi_0(\hat{y}) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \quad (2.54)$$

For treating the a_K term, the Taylor expansion from equation (2.45) is used:

$$\nabla_y G(T_t(\hat{x}), T_t(\hat{y})) = \nabla_y G(\hat{x}, \hat{y}) + t \kappa(\hat{x}, \hat{y}) + O(t^2). \quad (2.55)$$

Plugging in the above expansion and using eq. (2.36) and (2.39) we get:

$$= \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) (\nabla_y G(\hat{x}, \hat{y}) + t \kappa(\hat{x}, \hat{y}) + O(t^2)) \cdot (\hat{\mathbf{n}}(\hat{y}) + t A(\hat{y}) \hat{\mathbf{n}}(\hat{y}) + O(t^2)) \\ (g(\hat{y}) + t \nabla g(\hat{y}) \cdot \nu(\hat{y}) + O(t^2)) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \quad (2.56)$$

and the partial derivative at $t = 0$ is given as:

$$= \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{g(\hat{y}) \kappa(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) + g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (A(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\ + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) (\nabla g(\hat{y}) \cdot \nu(\hat{y}))\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \quad (2.57)$$

For the l term using eq. (2.39) we have:

$$= \int_{\Gamma_0} p(\hat{x}) (g(\hat{x}) + t \nabla g(\hat{x}) \cdot \nu(\hat{x}) + O(t^2)) d\Gamma_0(\hat{x}), \quad (2.58)$$

and the partial derivative at $t = 0$ is given as:

$$= \int_{\Gamma_0} p(\hat{x}) \nabla g(\hat{x}) \cdot \nu(\hat{x}) d\Gamma_0(\hat{x}). \quad (2.59)$$

Adding up individual terms to get the final shape gradient:

$$= \underbrace{\frac{1}{2} \int_{\Gamma_0} \Psi_0(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x})}_{\mathbf{T}_1} \\ + \underbrace{\int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \{ \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y}) \} p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})}_{\mathbf{T}_2} \\ - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) \kappa(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) + g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (A(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\ + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) (\nabla g(\hat{y}) \cdot \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ - \underbrace{\frac{1}{2} \int_{\Gamma_0} p(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x})}_{\mathbf{T}_4} \quad (2.60)$$

It is clear that the two pullback approaches presented yield the same formula for the shape gradient.

3 BEM shape gradient formula in 2D

3.1 Discussion about integrability

Assumptions: We assume that g is in $H^2(D)$ and ν is in $C^2(D)$. Assumptions on the velocity field ν are required for continuous second-order derivatives, which we will encounter while discussing the implementation. Assumptions on g are required for the following integral to be well defined, which we see in the shape

gradient formula from eq. (2.60) (In \mathbf{T}_1 and \mathbf{T}_4):

$$\int_{\Gamma} \Psi \nabla g \cdot \nu \, d\Gamma, \quad \Psi \in H^{-\frac{1}{2}}(\Gamma). \quad (3.1)$$

With g being in $H^2(D)$, ∇g lies in $H^1(D)$ and its restriction to the boundary lies in $H^{\frac{1}{2}}(\Gamma)$. This ensures the above integral to be well defined based on duality arguments [5, Ch. 1, Thm 1.3.37]. In \mathbf{T}_3 the $\nabla g \cdot \nu$ term is present in the variational form for the Double Layer BIO, which is well defined too with $g \in H^2(D)$. We focus on 2D where the fundamental solution is given as:

$$\begin{aligned} G(x, y) &= -\frac{1}{2\pi} \log \|x - y\|, \quad x, y \in \mathbb{R}^2, \\ \nabla_y G(x, y) &= -\nabla_x G(x, y) = \frac{1}{2\pi} \frac{x - y}{\|x - y\|^2}, \\ \kappa(x, y) &:= \frac{d(\nabla_y G(T_t(x), T_t(y)))}{dt} \Big|_{t=0} = \frac{1}{2\pi} \left(\frac{\nu(x) - \nu(y)}{\|x - y\|^2} - 2 \frac{(x - y)(x - y) \cdot (\nu(x) - \nu(y))}{\|x - y\|^4} \right). \end{aligned} \quad (3.2)$$

\mathbf{T}_1 and \mathbf{T}_4 in eq. (2.60) have the same structure as both $\Psi, p \in H^{-\frac{1}{2}}(\Gamma_0)$. Because of assumptions on g and ν , both integrals are well defined even for piecewise smooth boundaries. \mathbf{T}_2 and \mathbf{T}_3 need to be treated in some way as they contain singular functions in the integrand.

Using the fact $\nabla_x G(\hat{x}, \hat{y}) = -\nabla_y G(\hat{x}, \hat{y})$, \mathbf{T}_2 in eq. (2.60) gives :

$$\begin{aligned} &= \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) p(\hat{x}) \nabla_x G(\hat{x}, \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y})) \, d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ &= -\frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) p(\hat{x}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nu(\hat{x}) - \nu(\hat{y})) \, d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \end{aligned} \quad (3.3)$$

Using the following Taylor expansion:

$$\nu(\hat{x}) = \nu(\hat{y}) + \nabla \nu(\hat{y})^T (\hat{x} - \hat{y}) + O(\|\hat{x} - \hat{y}\|^2), \quad (3.4)$$

the highlighted singular part in equation (3.3) can be written as:

$$= \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y})^T (\hat{x} - \hat{y}) + O(\|\hat{x} - \hat{y}\|^2)). \quad (3.5)$$

From the Taylor expansion it is clear that the singular expression has a finite limit for $\hat{x} \rightarrow \hat{y}$ because of assumptions on ν and thus the highlighted expression in eq. (3.3) can be replaced by a function in $C^0(D)$. Thus the integral is well defined for all $\Psi, p \in H^{-\frac{1}{2}}(\Gamma_0)$, even for piecewise smooth boundaries. If $\nu \in C^\infty(D)$, the expression above is also $C^\infty(D)$ away from the line $\hat{x} = \hat{y}$.

\mathbf{T}_3 in eq. (2.60) has 3 components. The first component, using the expression for κ in eq. (3.2):

$$= \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - 2 \frac{(\hat{x} - \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) (\hat{x} - \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^4} \right\} \, d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \quad (3.6)$$

The expression within curly brackets highlighted above is singular for $\hat{x} = \hat{y}$. The second part of this expression is:

$$= \frac{(\hat{x} - \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})}{\|\hat{x} - \hat{y}\|^2} \frac{(\hat{x} - \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2}. \quad (3.7)$$

The first part of the expression above, highlighted in yellow, is the double layer kernel which is known to be well behaved even for piecewise smooth boundaries [5]. Using the result from equation (3.5), we see that the expression in eq. (3.7) has a finite limit for $\hat{x} \rightarrow \hat{y}$ and similar arguments follow where it can be replaced by

a function from $C^0(D)$. Thus the second part of the integral in eq. (3.6) is well defined for all $p \in H^{-\frac{1}{2}}(\Gamma_0)$, even for piecewise smooth boundaries.

First part of the integrand in equation (3.6) is given as:

$$= p(\hat{x}) g(\hat{y}) \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} = p(\hat{x}) g(\hat{y}) \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nabla \nu(\hat{y})^T (\hat{x} - \hat{y}) + O(\|\hat{x} - \hat{y}\|^2))}{\|\hat{x} - \hat{y}\|^2}. \quad (3.8)$$

For $\hat{x} \rightarrow \hat{y}$ this behaves as $O(\|\hat{x} - \hat{y}\|^{-1})$ and is not integrable.

Second part of \mathbf{T}_3 in eq. (2.60):

$$= \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (A(\hat{y}) \hat{\mathbf{n}}(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \quad (3.9)$$

Using the expression for the matrix A from eq. (2.36) we get:

$$= \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \nabla \cdot \nu(\hat{y}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \quad (3.10)$$

$$- \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \quad (3.11)$$

We see that the second part of \mathbf{T}_3 in (2.60) splits into two parts, one of which is like a Double Layer integral (3.10), which is well defined for all $p \in H^{-\frac{1}{2}}(\Gamma_0)$, even for smooth boundaries. The other part (3.11) behaves as $O(\|\hat{x} - \hat{y}\|^{-1})$ for $\hat{x} \rightarrow \hat{y}$ which is not integrable.

Third part of \mathbf{T}_3 in eq. (2.60) is again like double layer which is well behaved for all $p \in H^{-\frac{1}{2}}(\Gamma_0)$. As shown above in eq. (3.8) and (3.11), two terms appear with $O(\|x - y\|^{-1})$ behaviour. They are both obtained after simplifying the third term in eq. (2.60). These terms can be combined to get the following:

$$\begin{aligned} &= \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ &- \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\ &= \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \end{aligned} \quad (3.12)$$

Using the Taylor expansion from eq. (3.4), the above integral becomes:

$$= \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nabla \nu(\hat{y})^T (\hat{x} - \hat{y}) + O(\|\hat{x} - \hat{y}\|^2))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} p(\hat{x}) g(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}), \quad (3.13)$$

and the leading order term in the singular part of integrand is given as:

$$p(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nabla \nu(\hat{y})^T (\hat{x} - \hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} = 0. \quad (3.14)$$

Thus the $O(\|x - y\|^{-1})$ singularity cancels and we get an integrand which has a finite limit for $\hat{x} \rightarrow \hat{y}$. The singular expression can be replaced by a function in $C^0(D)$ and the integral is well defined for all $p \in H^{-\frac{1}{2}}(\Gamma_0)$, even for piecewise smooth boundaries.

Theorem 3.1. *The shape gradient given in eq. (2.60) is a continuous quadratic functional for all $\Psi, p \in H^{-\frac{1}{2}}(\Gamma_0)$ assuming $g \in H^2(D)$ and $\nu \in C^2(D)$, even for piecewise smooth boundaries.*

The formula for shape gradient in 2D is given as:

$$\begin{aligned}
&= \frac{1}{2} \underbrace{\int_{\Gamma_0} \Psi_0(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x})}_{\mathbf{T_I}} \\
&- \frac{1}{2\pi} \underbrace{\int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) p(\hat{x}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nu(\hat{x}) - \nu(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})}_{\mathbf{T_{II}}} \\
&- \frac{1}{2\pi} \underbrace{\int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})}_{\mathbf{T_{III}}} \\
&\frac{1}{2\pi} \underbrace{\int_{\Gamma_0} \int_{\Gamma_0} 2p(\hat{x}) g(\hat{y}) \left\{ \frac{(\hat{x} - \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) (\hat{x} - \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^4} \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})}_{\mathbf{T_{IV}}} \\
&- \frac{1}{2\pi} \underbrace{\int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \nabla \cdot \nu(\hat{y}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})}_{\mathbf{T_V}} \\
&- \frac{1}{2\pi} \underbrace{\int_{\Gamma_0} \int_{\Gamma_0} \left(\frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) \right) (\nabla g(\hat{y}) \cdot \nu(\hat{y})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})}_{\mathbf{T_{VI}}} \\
&- \frac{1}{2} \underbrace{\int_{\Gamma_0} p(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x})}_{\mathbf{T_{VII}}}
\end{aligned} \tag{3.15}$$

3.2 Evaluation of Shape Gradient formula in a discrete setting

3.2.1 Evaluating state and adjoint solution

The state and adjoint problems are solved numerically using a finite dimensional subspace $V_N \subset H^{-\frac{1}{2}}(\Gamma)$, which is the idea of a Galerkin approximation. Thus, these functions can be written as linear combination of the basis functions for the finite dimensional space V_N :

$$\Psi_0(\hat{x}) = \sum_{i=1}^N a_i \beta_i^N(\hat{x}), \quad p(\hat{x}) = \sum_{j=1}^N b_j \beta_j^N(\hat{x}). \tag{3.16}$$

The set $\{\beta_1, \beta_2, \dots, \beta_N\}$ is the set of ordered bases for the space V_N .

Next ingredient is the mesh of the boundary. The definition follows the lecture notes [5, Ch. 1, Sec 1.4.2], assuming that the boundary Γ_0 is a curved polygon:

$$\Gamma_0 = \cup_{j=1}^M \Gamma^j, \quad \Gamma^i \cap \Gamma^j = \phi. \tag{3.17}$$

The curved edges of this curved polygon are given by Γ^j which can be pulled back to a reference interval of $[-1,1]$ using a C^2 parametrization γ_j .

$$\gamma_j : [-1, 1] \rightarrow \Gamma^j. \tag{3.18}$$

For creating the mesh, this reference interval is partitioned as follows:

$$-1 := \zeta_0 < \zeta_1 < \dots < \zeta_{L-1} < \zeta_L := 1. \tag{3.19}$$

This gives us the vertices and panels:

$$\begin{aligned}
&\text{Vertices: } X_i^j = \gamma_j(\zeta_i), \quad i = 1, \dots, L, \quad j = 1, \dots, M. \\
&\text{Panels: } \pi_i^j = \gamma_j([\zeta_{i-1}, \zeta_i]), \quad i = 1, \dots, L, \quad j = 1, \dots, M. \\
&\mathcal{M} = \{\pi_i^j : \pi_i^j = \gamma_j([\zeta_{i-1}, \zeta_i]), \quad i = 1, \dots, L, \quad j = 1, \dots, M\}.
\end{aligned} \tag{3.20}$$

\mathcal{M} denotes the mesh which is the set of all the panels. Using the definition of the panels above, we can also define a parametrization of the panels on the reference interval $[-1,1]$:

$$\begin{aligned}\gamma_{\pi_i^j} &: [-1, 1] \rightarrow \pi_i^j, \\ \gamma_{\pi_i^j}(s) &= \gamma_j\left(\frac{(\zeta_{i-1} + \zeta_i)}{2} + s\frac{(\zeta_i - \zeta_{i-1})}{2}\right).\end{aligned}\tag{3.21}$$

Now, we define the boundary element spaces following the definition in the lecture notes [5, Ch. 1, eq. 1.4.22]. Since we are just dealing with functions in $H^{-\frac{1}{2}}(\Gamma_0)$, we only need the space $S_p^{-1}(\mathcal{M})$:

$$S_p^{-1}(\mathcal{M}) := \{v \in C^0(\Gamma_0) : \gamma_j^*(v|_\pi) \in \mathcal{P}_p, \forall \pi \in \mathcal{M}\}, p \geq 0.\tag{3.22}$$

We also know that for the functions from this space which are associated with a panel π , the support is just the panel π [5, Ch. 1, Sec. 1.4.27]. This will be useful when presenting the evaluation routines for the shape gradient. Also, the pullback of the basis functions under the panel parametrization of its supporting panel will give us a reference shape function. This mapping from the global shape function to the reference shape function depends only on the global shape function index and the panel index. If the support for a basis function $\beta_i^N(x)$ is the panel π :

$$\gamma_\pi^* \beta_i^N(s) = \hat{\beta}_k(s),\tag{3.23}$$

$\hat{\beta}_k$ is the k th reference shape function. The mapping $(k, \pi) \rightarrow i$ is unique [5, Ch. 1, Sec. 1.4.75]:

$$\text{locglobmap}(k, \pi) = i.\tag{3.24}$$

Local integrals are evaluated and then mapped to a global position dictated by the local to global map described above. The procedure for solving the state problem is laid out in the lecture notes [5, Ch. 1, Sec. 1.4.46] and is similar for the adjoint problem as the LHS in the variational equation is the same bilinear form a_V (Single Layer).

3.2.2 Evaluating \mathbf{T}_I and \mathbf{T}_{VII} in 2D shape gradient formula

It is assumed that g and ∇g are available in procedural form. For the velocity field, we assume that the first order and second order derivatives are available in procedural form.

Evaluation of the single integrals in the shape gradient formula is straightforward. \mathbf{T}_I in eq. (3.15) is given as:

$$\begin{aligned}&= \int_{\Gamma_0} \Psi_0(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\ &= \sum_{i=1}^N a_i \int_{\Gamma_0} \beta_i^N(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\ &= \sum_{i=1}^N a_i V_i, \quad V_i = \int_{\Gamma_0} \beta_i^N(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}).\end{aligned}\tag{3.25}$$

Let panel π be the support for the basis function β_i^N :

$$V_i = \int_{\pi} \beta_i^N(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}).\tag{3.26}$$

Using the parametrization for the panel, we get a local integral

$$= \int_{s=-1}^1 \hat{\beta}_k(s) \nabla g(\gamma_\pi(s)) \cdot \nu(\gamma_\pi(s)) \|\dot{\gamma}_\pi(s)\| ds.\tag{3.27}$$

$\hat{\beta}_k$ is a reference shape function such that $\text{locglobmap}(k, \pi) = i$. Evaluating these local integrals for all combinations of π and $\hat{\beta}_k$, and using the local to global map, we can evaluate the vector \mathbf{V} and hence the

final integral. Similarly, we can evaluate $\mathbf{T}_{\mathbf{VI}}$ in eq. (3.15):

$$\begin{aligned}
&= \int_{\Gamma_0} p(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
&= \sum_{i=1}^N b_i \int_{\Gamma_0} \beta_i^N(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
&= \sum_{i=1}^N b_i V_i, \quad V_i = \int_{\Gamma_0} \beta_i^N(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}).
\end{aligned} \tag{3.28}$$

The vector \mathbf{V} is same as for $\mathbf{T}_{\mathbf{I}}$. The final integral is evaluated by taking the dot product of the vector \mathbf{b} and \mathbf{V} .

3.2.3 Evaluating $\mathbf{T}_{\mathbf{II}}$ in 2D shape gradient formula

Evaluation of the double integrals in the shape gradient formula is a little more involved due to the presence of singular integrands. For the second term in eq. (3.15):

$$\begin{aligned}
&= \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) p(\hat{x}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nu(\hat{x}) - \nu(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= \sum_{i=1}^N \sum_{j=1}^N a_i b_j \int_{\Gamma_0} \int_{\Gamma_0} \beta_i^N(\hat{y}) \beta_j^N(\hat{x}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nu(\hat{x}) - \nu(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= \sum_{i=1}^N \sum_{j=1}^N a_i b_j R_{ij}, \quad R_{ij} = \int_{\Gamma_0} \int_{\Gamma_0} \beta_i^N(\hat{y}) \beta_j^N(\hat{x}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nu(\hat{x}) - \nu(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}).
\end{aligned} \tag{3.29}$$

Let the support for the basis functions β_i^N and β_j^N be π and π' respectively. Thus the term R_{ij} above can be written as:

$$\begin{aligned}
&= \int_{\pi} \int_{\pi'} \beta_i^N(\hat{y}) \beta_j^N(\hat{x}) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nu(\hat{x}) - \nu(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= \int_{t=-1}^1 \int_{s=-1}^1 \hat{\beta}_k(t) \hat{\beta}_l(s) \frac{\gamma_{\pi'}(s) - \gamma_{\pi}(t)}{\|\gamma_{\pi'}(s) - \gamma_{\pi}(t)\|^2} \cdot (\nu(\gamma_{\pi'}(s)) - \nu(\gamma_{\pi}(t))) \|\dot{\gamma}_{\pi'}(s)\| \|\dot{\gamma}_{\pi}(t)\| ds dt.
\end{aligned} \tag{3.30}$$

By evaluating the local integral above for all combinations of $\pi, \pi', \hat{\beta}_k$ and $\hat{\beta}_l$, and using the local to global mapping, we can find the matrix R_{ij} . If $\pi \cap \pi' = \{\Phi\}$, we are away from the singularity and the double integral can be evaluated in a straightforward manner using tensor product quadrature rule.

Coinciding panels: If $\pi = \pi'$ or the panels coincide, we have:

$$R_{ij} = \int_{t=-1}^1 \int_{s=-1}^1 \hat{\beta}_k(t) \hat{\beta}_l(s) \frac{\gamma_{\pi}(s) - \gamma_{\pi}(t)}{\|\gamma_{\pi}(s) - \gamma_{\pi}(t)\|^2} \cdot (\nu(\gamma_{\pi}(s)) - \nu(\gamma_{\pi}(t))) \|\dot{\gamma}_{\pi}(s)\| \|\dot{\gamma}_{\pi}(t)\| ds dt. \tag{3.31}$$

The integrand above has a singularity for $s = t$ but has a limit for $s \rightarrow t$. We rewrite the integral as:

$$\int_{t=-1}^1 \int_{s=-1}^1 \hat{\beta}_k(t) \hat{\beta}_l(s) f(s, t) \|\dot{\gamma}_{\pi}(s)\| \|\dot{\gamma}_{\pi}(t)\| ds dt. \tag{3.32}$$

Where $f(s, t)$ is a C^0 function defined as:

$$f(s, t) = \begin{cases} \frac{\dot{\gamma}_{\pi}(t) \cdot (\nabla \nu(\gamma_{\pi}(t)))^T \dot{\gamma}_{\pi}(t)}{\|\dot{\gamma}_{\pi}(t)\|^2} & \text{if } s = t \\ \frac{\gamma_{\pi}(s) - \gamma_{\pi}(t)}{\|\gamma_{\pi}(s) - \gamma_{\pi}(t)\|^2} \cdot (\nu(\gamma_{\pi}(s)) - \nu(\gamma_{\pi}(t))) & \text{otherwise.} \end{cases} \tag{3.33}$$

The value of $f(s, t)$ at $s = t$ is the limit for $s \rightarrow t$ found using Taylor expansions:

$$\begin{aligned} \gamma_\pi(s) &= \gamma_\pi(t) + (s-t)\dot{\gamma}_\pi(t) + \frac{(s-t)^2}{2}\ddot{\gamma}_\pi(t) + O((s-t)^3) \\ \implies \gamma_\pi(s) - \gamma_\pi(t) &= (s-t)\dot{\gamma}_\pi(t) + \frac{(s-t)^2}{2}\ddot{\gamma}_\pi(t) + O((s-t)^3) \\ \implies \|\gamma_\pi(s) - \gamma_\pi(t)\|^2 &= (s-t)^2(\|\dot{\gamma}_\pi(t)\|^2 + O(s-t)). \end{aligned} \quad (3.34)$$

Taylor expansion for the velocity field:

$$\begin{aligned} \nu(\gamma_\pi(s)) &= \nu(\gamma_\pi(t)) + (s-t)\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t) + O((s-t)^2) \\ \implies \nu(\gamma_\pi(s)) - \nu(\gamma_\pi(t)) &= (s-t)\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t) + O((s-t)^2). \end{aligned} \quad (3.35)$$

Using the Taylor expansions, the limit is calculated as:

$$\lim_{s \rightarrow t} \frac{\gamma_\pi(s) - \gamma_\pi(t)}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^2} \cdot (\nu(\gamma_\pi(s)) - \nu(\gamma_\pi(t))) \quad (3.36)$$

$$= \lim_{s \rightarrow t} \frac{(s-t)\dot{\gamma}_\pi(t) + O((s-t)^2)}{(s-t)^2(\|\dot{\gamma}_\pi(t)\|^2 + O((s-t)))} \cdot ((s-t)\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t) + O((s-t)^2)) \quad (3.37)$$

$$= \frac{\dot{\gamma}_\pi(t) \cdot (\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t))}{\|\dot{\gamma}_\pi(t)\|^2}. \quad (3.38)$$

$f(s, t)$ is bounded. Thus for coinciding panels R_{ij} can be evaluated by quadrature.

Adjacent panels: For the case $\pi \cap \pi' = P$, or adjacent panels, with P being the common point, we evaluate R_{ij} as follows: First we require a local arclength parametrization for the panels π and π' :

$$\begin{aligned} K(t') &: [0, |\pi|] \rightarrow \pi, \\ K'(s') &: [0, |\pi'|] \rightarrow \pi'. \end{aligned} \quad (3.39)$$

The local arclength parametrizations satisfy $K(0) = K'(0) = P$ and $\|\dot{K}(0)\| = \|\dot{K}'(0)\| = 1$. Assuming $\gamma_\pi(1) = \gamma_{\pi'}(-1)$, the local arclength parametrization and the panel parametrizations are related to each other as follows:

$$K(t') = \gamma_\pi(1 - \frac{2t'}{|\pi|}), \quad K'(s') = \gamma_{\pi'}(\frac{2s'}{|\pi'|} - 1). \quad (3.40)$$

Note: Similar relation can be established if $\gamma_\pi(-1) = \gamma_{\pi'}(1)$. In the implementation we check for the assumption $\gamma_\pi(1) = \gamma_{\pi'}(-1)$.

Thus we can transform the local integral in eq. (3.30) to arclength parametrizations by using the coordinate transformation:

$$t = 1 - \frac{2t'}{|\pi|}, \quad s = \frac{2s'}{|\pi'|} - 1. \quad (3.41)$$

Using the coordinate transformation mentioned above and renaming s' and t' to s and t respectively, the local integral becomes :

$$\begin{aligned} &= \frac{4}{|\pi||\pi'|} \int_{t=0}^{|\pi|} \int_{s=0}^{|\pi'|} \hat{\beta}_k(1 - \frac{2t}{|\pi|}) \hat{\beta}_l(\frac{2s}{|\pi'|} - 1) \|\dot{\gamma}_\pi(1 - \frac{2t}{|\pi|})\| \|\dot{\gamma}_{\pi'}(\frac{2s}{|\pi'|} - 1)\| \\ &\quad \frac{K'(s) - K(t)}{\|K'(s) - K(t)\|^2} \cdot (\nu(K'(s)) - \nu(K(t))) \, ds \, dt. \end{aligned} \quad (3.42)$$

To treat the singular term highlighted above, we use Taylor expansions about the point 0 as the singularity occurs when $s = t = 0$:

$$\begin{aligned} K(t) &= K(0) + t\dot{K}(0) + O(t^2), \\ K'(s) &= K'(0) + s\dot{K}'(0) + O(s^2). \\ \implies K'(s) - K(t) &= s\dot{K}'(0) - t\dot{K}(0) + O(s^2 + t^2) \\ \implies \|K'(s) - K(t)\|^2 &= s^2 + t^2 - 2st\dot{K}(0) \cdot \dot{K}'(0) + O(s^4 + t^4). \end{aligned} \quad (3.43)$$

Taylor expansion for the velocity field:

$$\begin{aligned}
\nu(K(t)) &= \nu(K(0)) + t\nabla\nu(K(0))^T \dot{K}(0) + \frac{t^2}{2}(\nabla\nu(K(0))^T \ddot{K}(0) + M(0)\dot{K}(0)) + O(t^3), \\
M(t) &:= \frac{d(\nabla\nu(K(t))^T)}{dt}. \\
\nu(K'(s)) &= \nu(K'(0)) + s\nabla\nu(K'(0))^T \dot{K}'(0) + \frac{s^2}{2}(\nabla\nu(K'(0))^T \ddot{K}'(0) + M'(0)\dot{K}'(0)) + O(s^3), \\
M'(s) &:= \frac{d(\nabla\nu(K'(s))^T)}{ds}. \\
\nu(K'(s)) - \nu(K(t)) &= s\nabla\nu(K'(0))^T \dot{K}'(0) - t\nabla\nu(K(0))^T \dot{K}(0) + O(s^2 + t^2).
\end{aligned} \tag{3.44}$$

Due to the presence of $s^2 + t^2$, we use polar coordinates:

$$s = r \cos(\phi), \quad t = r \sin(\phi). \tag{3.45}$$

Using Taylor expansions given above, the highlighted term in eq. (3.42):

$$\begin{aligned}
&= \frac{K'(s) - K(t)}{\|K'(s) - K(t)\|^2} \cdot (\nu(K'(s)) - \nu(K(t))) \\
&= \frac{s\dot{K}'(0) - t\dot{K}(0) + O(s^2 + t^2)}{s^2 + t^2 - 2st\dot{K}(0) \cdot \dot{K}'(0) + O(s^4 + t^4)} \cdot (s\nabla\nu(K'(0))^T \dot{K}'(0) - t\nabla\nu(K(0))^T \dot{K}(0) + O(s^2 + t^2)) \\
&= \frac{r \cos(\phi)\dot{K}'(0) - r \sin(\phi)\dot{K}(0) + O(r^2)}{r^2 - r^2 \sin(2\phi)\dot{K}(0) \cdot \dot{K}'(0) + O(r^4)} \cdot (r \cos(\phi)\nabla\nu(K'(0))^T \dot{K}'(0) - r \sin(\phi)\nabla\nu(K(0))^T \dot{K}(0) + O(r^2)).
\end{aligned} \tag{3.46}$$

For $r \rightarrow 0$:

$$= \frac{\cos(\phi)\dot{K}'(0) - \sin(\phi)\dot{K}(0)}{1 - \sin(2\phi)\dot{K}(0) \cdot \dot{K}'(0)} \cdot (\cos(\phi)\nabla\nu(K'(0))^T \dot{K}'(0) - \sin(\phi)\nabla\nu(K(0))^T \dot{K}(0)). \tag{3.47}$$

We replace the singular term highlighted in eq. (3.42) with the C^0 function $D(r, \phi)$ defined as:

$$D(r, \phi) = \begin{cases} \frac{K'(r \cos(\phi)) - K(r \sin(\phi))}{\|K'(r \cos(\phi)) - K(r \sin(\phi))\|^2} \cdot (\nu(K'(r \cos(\phi))) - \nu(K(r \sin(\phi)))) & r > 0 \\ \frac{\cos(\phi)\dot{K}'(0) - \sin(\phi)\dot{K}(0)}{1 - \sin(2\phi)\dot{K}(0) \cdot \dot{K}'(0)} \cdot (\cos(\phi)\nabla\nu(K'(0))^T \dot{K}'(0) - \sin(\phi)\nabla\nu(K(0))^T \dot{K}(0)) & r = 0 \end{cases} \tag{3.48}$$

After the local arclength transformation followed by polar coordinate transformation, the local integral is in the following form:

$$\int_{\phi=0}^{\arctan(\frac{|\pi|}{|\pi|})} \int_{r=0}^{\frac{|\pi|}{\cos(\phi)}} \mathcal{F}(r, \phi) D(r, \phi) dr d\phi + \int_{\phi=\arctan(\frac{|\pi|}{|\pi|})}^{\frac{\pi}{2}} \int_{r=0}^{\frac{|\pi|}{\sin(\phi)}} \mathcal{F}(r, \phi) D(r, \phi) dr d\phi. \tag{3.49}$$

With both $\mathcal{F}(r, \phi)$ and $D(r, \phi)$ being continuous, the local integral can be evaluated by tensor product quadrature rule.

3.2.4 Evaluating T_{III} in 2D shape gradient formula

The third term in eq. (3.15):

$$\begin{aligned}
&= \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= \sum_{i=1}^N \frac{b_i}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= \sum_{i=1}^N b_i S_i, \\
S_i &= \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}).
\end{aligned} \tag{3.50}$$

Let panel π be the support of the basis function β_i^N .

$$S_i = \frac{1}{2\pi} \int_{\Gamma_0} \int_{\pi} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \tag{3.51}$$

The outer integral is over the whole boundary but it can be broken down into the sum of integrals over individual panels:

$$S_i = \sum_{\pi' \in \mathcal{M}} \frac{1}{2\pi} \left(\int_{\pi'} \int_{\pi} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \right). \tag{3.52}$$

The local integral in this case is given as:

$$\begin{aligned}
&= \int_{\pi'} \int_{\pi} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{\hat{\mathbf{n}}(\hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^2} - \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= \int_{t=-1}^1 \int_{s=-1}^1 \hat{\beta}_k(s) g(\gamma_{\pi'}(t)) \left\{ \frac{\hat{\mathbf{n}}(\gamma_{\pi'}(t)) \cdot (\nu(\gamma_{\pi}(s)) - \nu(\gamma_{\pi'}(t)))}{\|\gamma_{\pi}(s) - \gamma_{\pi'}(t)\|^2} \right. \\
&\quad \left. - \frac{\gamma_{\pi}(s) - \gamma_{\pi'}(t)}{\|\gamma_{\pi}(s) - \gamma_{\pi'}(t)\|^2} \cdot (\nabla \nu(\gamma_{\pi'}(t)) \hat{\mathbf{n}}(\gamma_{\pi'}(t))) \right\} \|\dot{\gamma}_{\pi}(s)\| \|\dot{\gamma}_{\pi'}(t)\| ds dt.
\end{aligned} \tag{3.53}$$

If $\pi' \cap \pi = \{\phi\}$, we are away from the singularity and can use tensor product quadrature rule to evaluate the integral.

Coinciding panels: If the panels coincide, that is $\pi' = \pi$, the integral becomes:

$$\begin{aligned}
&= \int_{t=-1}^1 \int_{s=-1}^1 \hat{\beta}_k(s) g(\gamma_{\pi}(t)) \left\{ \frac{\hat{\mathbf{n}}(\gamma_{\pi}(t)) \cdot (\nu(\gamma_{\pi}(s)) - \nu(\gamma_{\pi}(t)))}{\|\gamma_{\pi}(s) - \gamma_{\pi}(t)\|^2} \right. \\
&\quad \left. - \frac{\gamma_{\pi}(s) - \gamma_{\pi}(t)}{\|\gamma_{\pi}(s) - \gamma_{\pi}(t)\|^2} \cdot (\nabla \nu(\gamma_{\pi}(t)) \hat{\mathbf{n}}(\gamma_{\pi}(t))) \right\} \|\dot{\gamma}_{\pi}(s)\| \|\dot{\gamma}_{\pi}(t)\| ds dt.
\end{aligned} \tag{3.54}$$

The expression within curly brackets highlighted above is singular for $s = t$, but has a limit as shown in eq. (3.14). Using Taylor expansions in eq. (3.35), we replace the function within curly brackets with the following C^0 function:

$$F(s, t) = \begin{cases} \frac{\hat{\mathbf{n}}(\gamma_{\pi}(t)) \cdot (\nu(\gamma_{\pi}(s)) - \nu(\gamma_{\pi}(t)))}{\|\gamma_{\pi}(s) - \gamma_{\pi}(t)\|^2} - \frac{\gamma_{\pi}(s) - \gamma_{\pi}(t)}{\|\gamma_{\pi}(s) - \gamma_{\pi}(t)\|^2} \cdot (\nabla \nu(\gamma_{\pi}(t)) \hat{\mathbf{n}}(\gamma_{\pi}(t))) & s \neq t \\ \frac{1}{2} \frac{\hat{\mathbf{n}}(\gamma_{\pi}(t)) \cdot (\chi(t) \dot{\gamma}_{\pi}(t))}{\|\dot{\gamma}_{\pi}(t)\|^2} & s = t, \end{cases} \tag{3.55}$$

where $\chi(t)$ is defined as:

$$\chi(t) := \frac{d(D\nu(\gamma_\pi(t)))}{dt}. \quad (3.56)$$

The limit for the highlighted expression for $s \rightarrow t$ is obtained using Taylor expansions as follows:

$$\begin{aligned} &= \frac{\hat{\mathbf{n}}(\gamma_\pi(t)) \cdot (\nu(\gamma_\pi(s)) - \nu(\gamma_\pi(t)))}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^2} - \frac{\gamma_\pi(s) - \gamma_\pi(t)}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^2} \cdot (\nabla\nu(\gamma_\pi(t))\hat{\mathbf{n}}(\gamma_\pi(t))) \\ &= \frac{\hat{\mathbf{n}}(\gamma_\pi(t)) \cdot ((s-t)\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t) + \frac{(s-t)^2}{2}(\nabla\nu(\gamma_\pi(t))^T\ddot{\gamma}_\pi(t) + \chi(t)\dot{\gamma}_\pi(t)) + O((s-t)^3))}{(s-t)^2(\|\dot{\gamma}_\pi(t)\|^2 + O((s-t)))} \\ &\quad - \frac{(s-t)\dot{\gamma}_\pi(t) + \frac{(s-t)^2}{2}\ddot{\gamma}_\pi(t) + O((s-t)^3)}{(s-t)^2(\|\dot{\gamma}_\pi(t)\|^2 + O((s-t)))} \cdot (\nabla\nu(\gamma_\pi(t))\hat{\mathbf{n}}(\gamma_\pi(t))) \\ &= \frac{\hat{\mathbf{n}}(\gamma_\pi(t)) \cdot (\frac{(s-t)^2}{2}(\nabla\nu(\gamma_\pi(t))^T\ddot{\gamma}_\pi(t) + \chi(t)\dot{\gamma}_\pi(t)) + O((s-t)^3))}{(s-t)^2(\|\dot{\gamma}_\pi(t)\|^2 + O((s-t)))} \\ &\quad - \frac{\frac{(s-t)^2}{2}\ddot{\gamma}_\pi(t) + O((s-t)^3)}{(s-t)^2(\|\dot{\gamma}_\pi(t)\|^2 + O((s-t)))} \cdot (\nabla\nu(\gamma_\pi(t))\hat{\mathbf{n}}(\gamma_\pi(t))). \end{aligned} \quad (3.57)$$

For $s \rightarrow t$:

$$\begin{aligned} &= \frac{1}{2} \frac{\hat{\mathbf{n}}(\gamma_\pi(t)) \cdot (\nabla\nu(\gamma_\pi(t))^T\ddot{\gamma}_\pi(t) + \chi(t)\dot{\gamma}_\pi(t))}{\|\dot{\gamma}_\pi(t)\|^2} - \frac{1}{2} \frac{\ddot{\gamma}_\pi(t)}{\|\dot{\gamma}_\pi(t)\|^2} \cdot (\nabla\nu(\gamma_\pi(t))\hat{\mathbf{n}}(\gamma_\pi(t))) \\ &= \frac{1}{2} \frac{\hat{\mathbf{n}}(\gamma_\pi(t)) \cdot (\chi(t)\dot{\gamma}_\pi(t))}{\|\dot{\gamma}_\pi(t)\|^2}. \end{aligned} \quad (3.58)$$

Thus the integral can be evaluated using tensor product quadrature rule as the function $F(s, t)$ and the rest of the integrand is continuous.

Adjacent panels: For the case of adjacent panels or $\pi \cap \pi' = \{P\}$, we follow a similar procedure with local arclength parametrization of the panels introduced in eq. (3.39):

$$\begin{aligned} K(s') &: [0, |\pi|] \rightarrow \pi, \\ K'(t') &: [0, |\pi'|] \rightarrow \pi'. \end{aligned} \quad (3.59)$$

The parametrizations are such that $K(0) = K'(0) = P$ and $\|\dot{K}(0)\| = \|\dot{K}'(0)\| = 1$. Assuming $\gamma_\pi(1) = \gamma_{\pi'}(-1)$, we can transform the local integral in eq. (3.53) to arclength parametrizations by using the coordinate transformations:

$$t = \frac{2t'}{|\pi'|} - 1, \quad s = 1 - \frac{2s'}{|\pi|}. \quad (3.60)$$

After Renaming s' and t' to s and t respectively, we get:

$$\begin{aligned} &= \frac{4}{|\pi||\pi'|} \int_{t=0}^{|\pi'|} \int_{s=0}^{|\pi|} \hat{\beta}_k(1 - \frac{2s}{|\pi|}) g(K'(t)) \left\{ \frac{\hat{\mathbf{n}}(K'(t)) \cdot (\nu(K(s)) - \nu(K'(t)))}{\|K(s) - K'(t)\|^2} \right. \\ &\quad \left. - \frac{K(s) - K'(t)}{\|K(s) - K'(t)\|^2} \cdot (\nabla\nu(K'(t))\hat{\mathbf{n}}(K'(t))) \right\} \|\dot{\gamma}_\pi(1 - \frac{2s}{|\pi|})\| \|\dot{\gamma}_{\pi'}(\frac{2t}{|\pi'|} - 1)\| ds dt. \end{aligned} \quad (3.61)$$

The singular part of the integrand highlighted above within curly brackets:

$$= \frac{\hat{\mathbf{n}}(K'(t)) \cdot (\nu(K(s)) - \nu(K'(t)))}{\|K(s) - K'(t)\|^2} - \frac{K(s) - K'(t)}{\|K(s) - K'(t)\|^2} \cdot (\nabla\nu(K'(t))\hat{\mathbf{n}}(K'(t))). \quad (3.62)$$

Using the Taylor expansions about $s = 0$ and $t = 0$, presented in eq. (3.44), we get:

$$\begin{aligned}
&= \left\{ \hat{\mathbf{n}}(K'(t)) \cdot (s \nabla \nu(K(0))^T \dot{K}(0) + \frac{s^2}{2} (\nabla \nu(K(0))^T \ddot{K}(0) + M(0) \dot{K}(0))) \right. \\
&\quad - t \nabla \nu(K'(0))^T \dot{K}'(0) - \frac{t^2}{2} (\nabla \nu(K'(0))^T \ddot{K}'(0) + M'(0) \dot{K}'(0)) + O(s^3 + t^3) \\
&\quad \left. - (s \dot{K}(0) - t \dot{K}'(0) + \frac{s^2}{2} \ddot{K}(0) - \frac{t^2}{2} \ddot{K}'(0) + O(s^3 + t^3)) \cdot ((\nabla \nu(K'(0)) + t M'(0)^T + O(t^2)) \hat{\mathbf{n}}(K'(t))) \right\} \\
&/ (s^2 + t^2 - 2st \dot{K}(0) \cdot \dot{K}'(0) + O(s^4 + t^4)) \\
&= \frac{\hat{\mathbf{n}}(K'(t)) \cdot (\frac{s^2}{2} M(0) \dot{K}(0) + \frac{t^2}{2} M'(0) \dot{K}'(0) - st M'(0) \dot{K}(0) + \text{cubic terms})}{s^2 + t^2 - 2st \dot{K}(0) \cdot \dot{K}'(0) + O(s^4 + t^4)}.
\end{aligned}$$

Due to the presence of s^2 and t^2 , we use polar coordinates:

$$s = r \cos(\phi), \quad t = r \sin(\phi). \quad (3.63)$$

Using polar coordinates, we get:

$$= \frac{\hat{\mathbf{n}}(K'(r \sin(\phi))) \cdot (\frac{r^2}{2} \cos^2(\phi) M(0) \dot{K}(0) + \frac{r^2}{2} \sin^2(\phi) M'(0) \dot{K}'(0) - r^2 \sin(\phi) \cos(\phi) M'(0) \dot{K}(0) + O(r^3))}{r^2 - 2r^2 \sin(\phi) \cos(\phi) \dot{K}(0) \cdot \dot{K}'(0) + O(r^4)}. \quad (3.64)$$

for $r \rightarrow 0$, we get:

$$= \frac{\hat{\mathbf{n}}(K'(0)) \cdot (\frac{1}{2} \cos^2(\phi) M(0) \dot{K}(0) + \frac{1}{2} \sin^2(\phi) M'(0) \dot{K}'(0) - \sin(\phi) \cos(\phi) M'(0) \dot{K}(0))}{1 - \sin(2\phi) \dot{K}(0) \cdot \dot{K}'(0)}. \quad (3.65)$$

We treat the singular part highlighted above by switching to polar coordinates and replacing it with the following C^0 function:

$$Q(r, \phi) = \begin{cases} \frac{\hat{\mathbf{n}}(K'(r \sin(\phi))) \cdot (\nu(K(r \cos(\phi))) - \nu(K'(r \sin(\phi))))}{\|K(r \cos(\phi)) - K'(r \sin(\phi))\|^2} \\ - \frac{K(r \cos(\phi)) - K'(r \sin(\phi))}{\|K(r \cos(\phi)) - K'(r \sin(\phi))\|^2} \cdot (\nabla \nu(K'(r \sin(\phi))) \hat{\mathbf{n}}(K'(r \sin(\phi)))) & r \neq 0 \\ \frac{\hat{\mathbf{n}}(K'(0)) \cdot (\frac{1}{2} \cos^2(\phi) M(0) \dot{K}(0) + \frac{1}{2} \sin^2(\phi) M'(0) \dot{K}'(0) - \sin(\phi) \cos(\phi) M'(0) \dot{K}(0))}{1 - \sin(2\phi) \dot{K}(0) \cdot \dot{K}'(0)} & r = 0. \end{cases} \quad (3.66)$$

Local arclength transformation followed by the polar coordinate transformation gives us the local integral from eq. (3.61) in the following form:

$$\int_{\phi=0}^{\arctan(\frac{|\pi'|}{|\pi|})} \int_{r=0}^{\frac{|\pi|}{\cos(\phi)}} \mathcal{F}(r, \phi) Q(r, \phi) dr d\phi + \int_{\phi=\arctan(\frac{|\pi'|}{|\pi|})}^{\frac{\pi}{2}} \int_{r=0}^{\frac{|\pi'|}{\sin(\phi)}} \mathcal{F}(r, \phi) Q(r, \phi) dr d\phi. \quad (3.67)$$

As both $\mathcal{F}(r, \phi)$ and $Q(r, \phi)$ are continuous, we can evaluate the integral using tensor product quadrature rule.

3.2.5 Evaluating T_{IV} in the 2D shape gradient formula

The fourth term in eq. (3.15) is given as:

$$= \frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} 2p(\hat{x}) g(\hat{y}) \left\{ \frac{(\hat{x} - \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) (\hat{x} - \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^4} \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}). \quad (3.68)$$

Plugging in the formula for $p(\hat{x})$ from eq. (3.16), we get:

$$\begin{aligned}
&= \sum_{i=1}^N b_i \frac{1}{\pi} \int_{\Gamma_0} \int_{\Gamma_0} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{(\hat{x} - \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) (\hat{x} - \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^4} \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= \frac{1}{\pi} \sum_{i=1}^N b_i T_i, \\
T_i &= \int_{\Gamma_0} \int_{\Gamma_0} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{(\hat{x} - \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) (\hat{x} - \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^4} \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}).
\end{aligned} \tag{3.69}$$

Let panel π be the support for the basis function β_i^N :

$$\begin{aligned}
T_i &= \int_{\Gamma_0} \int_{\pi} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{(\hat{x} - \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) (\hat{x} - \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^4} \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= \sum_{\pi' \in \mathcal{M}} \int_{\pi'} \int_{\pi} \beta_i^N(\hat{x}) g(\hat{y}) \left\{ \frac{(\hat{x} - \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) (\hat{x} - \hat{y}) \cdot (\nu(\hat{x}) - \nu(\hat{y}))}{\|\hat{x} - \hat{y}\|^4} \right\} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}).
\end{aligned}$$

Integral inside the summation gives us the following local integral:

$$\begin{aligned}
&= \int_{t=-1}^1 \int_{s=-1}^1 \left\{ \frac{(\gamma_\pi(s) - \gamma_{\pi'}(t)) \cdot \hat{\mathbf{n}}(\gamma_{\pi'}(t)) (\gamma_\pi(s) - \gamma_{\pi'}(t)) \cdot (\nu(\gamma_\pi(s)) - \nu(\gamma_{\pi'}(t)))}{\|\gamma_\pi(s) - \gamma_{\pi'}(t)\|^4} \right\} \\
&\quad \hat{\beta}_k(s) g(\gamma_{\pi'}(t)) \|\dot{\gamma}_\pi(s)\| \|\dot{\gamma}_{\pi'}(t)\| ds dt. \tag{3.70}
\end{aligned}$$

Evaluating the local integral above for all combinations of π , π' and $\hat{\beta}_k$ and using local to global mapping, we can get the vector T . When $\pi \cap \pi' = \{\phi\}$, we are away from the singularity and the integral can be evaluated using tensor product quadrature rule.

Coinciding panels: When $\pi = \pi'$ or the panels coincide, the local integral becomes:

$$\begin{aligned}
&\int_{t=-1}^1 \int_{s=-1}^1 \left\{ \frac{(\gamma_\pi(s) - \gamma_\pi(t)) \cdot \hat{\mathbf{n}}(\gamma_\pi(t)) (\gamma_\pi(s) - \gamma_\pi(t)) \cdot (\nu(\gamma_\pi(s)) - \nu(\gamma_\pi(t)))}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^4} \right\} \\
&\quad \hat{\beta}_k(s) g(\gamma_\pi(t)) \|\dot{\gamma}_\pi(s)\| \|\dot{\gamma}_\pi(t)\| ds dt. \tag{3.71}
\end{aligned}$$

The integrand outside the curly brackets is analytic but the part inside is singular for $s = t$. As shown earlier there is a limit for the singular part which is evaluated using Taylor expansions from eq. (3.35). The highlighted expression above is written as:

$$\begin{aligned}
&= \frac{(\gamma_\pi(s) - \gamma_\pi(t)) \cdot \hat{\mathbf{n}}(\gamma_\pi(t)) (\gamma_\pi(s) - \gamma_\pi(t)) \cdot (\nu(\gamma_\pi(s)) - \nu(\gamma_\pi(t)))}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^4} \\
&= \frac{(\gamma_\pi(s) - \gamma_\pi(t)) \cdot \hat{\mathbf{n}}(\gamma_\pi(t)) (\gamma_\pi(s) - \gamma_\pi(t)) \cdot (\nu(\gamma_\pi(s)) - \nu(\gamma_\pi(t)))}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^2 \|\gamma_\pi(s) - \gamma_\pi(t)\|^2}.
\end{aligned} \tag{3.72}$$

Taylor expansion for the first part of the expression above:

$$\begin{aligned}
&= \frac{(\gamma_\pi(s) - \gamma_\pi(t)) \cdot \hat{\mathbf{n}}(\gamma_\pi(t))}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^2} \\
&= \frac{((s-t)\dot{\gamma}_\pi(t) + \frac{(s-t)^2}{2}\ddot{\gamma}_\pi(t) + O((s-t)^3)) \cdot \hat{\mathbf{n}}(\gamma_\pi(t))}{(s-t)^2 \|\dot{\gamma}_\pi(t)\|^2 + O((s-t)^3)} \\
&= \frac{\frac{(s-t)^2}{2}\ddot{\gamma}_\pi(t) + O((s-t)^3) \cdot \hat{\mathbf{n}}(\gamma_\pi(t))}{(s-t)^2 \|\dot{\gamma}_\pi(t)\|^2 + O((s-t)^3)}, \quad \dot{\gamma}_\pi(t) \cdot \hat{\mathbf{n}}(\gamma_\pi(t)) = 0.
\end{aligned} \tag{3.73}$$

The limit for $s \rightarrow t$:

$$= \frac{\ddot{\gamma}_\pi(t) \cdot \hat{\mathbf{n}}(\gamma_\pi(t))}{2\|\dot{\gamma}_\pi(t)\|^2}. \tag{3.74}$$

For the second part of the expression in eq. (3.72):

$$\begin{aligned}
&= \frac{(\gamma_\pi(s) - \gamma_\pi(t)) \cdot (\nu(\gamma_\pi(s)) - \nu(\gamma_\pi(t)))}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^2} \\
&= \frac{\left((s-t)\dot{\gamma}_\pi(t) + \frac{(s-t)^2}{2}\ddot{\gamma}_\pi(t) + O((s-t)^3) \right) \cdot \left((s-t)\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t) + O((s-t)^2) \right)}{(s-t)^2\|\dot{\gamma}_\pi(t)\|^2 + O((s-t)^3)}.
\end{aligned} \tag{3.75}$$

The limit for $s \rightarrow t$:

$$= \frac{\dot{\gamma}_\pi(t) \cdot (\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t))}{\|\dot{\gamma}_\pi(t)\|^2}. \tag{3.76}$$

Combining the results, we get the limit for the complete expression in eq. (3.72), for $s \rightarrow t$ as:

$$= \frac{(\ddot{\gamma}_\pi(t) \cdot \hat{\mathbf{n}}(\gamma_\pi(t))) \dot{\gamma}_\pi(t) \cdot (\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t))}{2\|\dot{\gamma}_\pi(t)\|^4}. \tag{3.77}$$

Replacing the singular part of the integrand with the following C^0 function:

$$C(s, t) = \begin{cases} \frac{(\gamma_\pi(s) - \gamma_\pi(t)) \cdot \hat{\mathbf{n}}(\gamma_\pi(t)) (\gamma_\pi(s) - \gamma_\pi(t)) \cdot (\nu(\gamma_\pi(s)) - \nu(\gamma_\pi(t)))}{\|\gamma_\pi(s) - \gamma_\pi(t)\|^4} & s \neq t \\ \frac{(\ddot{\gamma}_\pi(t) \cdot \hat{\mathbf{n}}(\gamma_\pi(t))) \dot{\gamma}_\pi(t) \cdot (\nabla\nu(\gamma_\pi(t))^T\dot{\gamma}_\pi(t))}{2\|\dot{\gamma}_\pi(t)\|^4} & s = t. \end{cases} \tag{3.78}$$

We can integrate eq. (3.71) as $C(s, t)$ is continuous along with the rest of the integrand.

Adjacent panels: For the case of adjacent panels or $\pi \cap \pi' = \{P\}$, we use local arclength parametrizations introduced in eq. (3.59):

$$\begin{aligned}
K(s') &: [0, |\pi|] \rightarrow \pi, \\
K'(t') &: [0, |\pi'|] \rightarrow \pi'.
\end{aligned} \tag{3.79}$$

The parametrizations are such that $K(0) = K'(0) = P$ and $\|\dot{K}(0)\| = \|\dot{K}'(0)\| = 1$. Assuming $\gamma_\pi(1) = \gamma_{\pi'}(-1)$, we can transform the local integral in eq. (3.70) to arclength parametrizations by using the coordinate transformations:

$$t = \frac{2t'}{|\pi'|} - 1, \quad s = 1 - \frac{2s'}{|\pi|}. \tag{3.80}$$

After Renaming s' and t' to s and t respectively, the local integral becomes:

$$\begin{aligned}
&= \frac{4}{|\pi||\pi'|} \int_{t=0}^{|\pi'|} \int_{s=0}^{|\pi|} \left\{ \frac{(K(s) - K'(t)) \cdot \hat{\mathbf{n}}(K'(t)) (K(s) - K'(t)) \cdot (\nu(K(s)) - \nu(K'(t)))}{\|K(s) - K'(t)\|^4} \right\} \\
&\quad \hat{\beta}_k \left(1 - \frac{2s}{|\pi|}\right) g(K'(t)) \|\dot{\gamma}_\pi \left(1 - \frac{2s}{|\pi|}\right)\| \|\dot{\gamma}_{\pi'} \left(\frac{2t}{|\pi'|} - 1\right)\| ds dt.
\end{aligned} \tag{3.81}$$

The singular part of the integrand highlighted above:

$$= \frac{(K(s) - K'(t)) \cdot \hat{\mathbf{n}}(K'(t)) (K(s) - K'(t)) \cdot (\nu(K(s)) - \nu(K'(t)))}{\|K(s) - K'(t)\|^2 \|K(s) - K'(t)\|^2}. \tag{3.82}$$

Using Taylor expansions from eq. (3.44), the expression above:

$$\begin{aligned}
&= (s\dot{K}(0) - t\dot{K}'(0) + O(s^2 + t^2)) \cdot \hat{\mathbf{n}}(K'(t)) \\
&\quad \times \left((s\dot{K}(0) - t\dot{K}'(0) + O(s^2 + t^2)) \cdot (s\nabla\nu(K(0))^T\dot{K}(0) - t\nabla\nu(K'(0))^T\dot{K}'(0) + O(s^2 + t^2)) \right) \\
&\quad / (s^2 + t^2 - 2st\dot{K}(0) \cdot \dot{K}'(0) + \text{cubic terms})^2.
\end{aligned} \tag{3.83}$$

Due to the presence of $s^2 + t^2$, we use polar coordinates $s = r \cos(\phi), t = r \sin(\phi)$. The expression above becomes:

$$\begin{aligned}
&= (r \cos(\phi) \dot{K}(0) - r \sin(\phi) \dot{K}'(0) + O(r^2)) \cdot \hat{\mathbf{n}}(K'(r \sin(\phi))) \\
&\quad \times \left((r \cos(\phi) \dot{K}(0) - r \sin(\phi) \dot{K}'(0) + O(r^2)) \cdot (r \cos(\phi) \nabla \nu(K(0))^T \dot{K}(0) - r \sin(\phi) \nabla \nu(K'(0))^T \dot{K}'(0) + O(r^2)) \right) \\
&\quad / (r^2 - r^2 \sin(2\phi) \dot{K}(0) \cdot \dot{K}'(0) + O(r^3))^2 .
\end{aligned} \tag{3.84}$$

The expression above is still $O(\frac{1}{r})$ but when making the polar coordinate transformations, we get a Jacobian equal to r . Thus multiplying the expression above by the Jacobian gets rid of the $\frac{1}{r}$ singularity. The limit for the expression as $r \rightarrow 0$, including the Jacobian r is:

$$\begin{aligned}
&= (\cos(\phi) \dot{K}(0) - \sin(\phi) \dot{K}'(0)) \cdot \hat{\mathbf{n}}(K'(0)) \\
&\quad \times \left((\cos(\phi) \dot{K}(0) - \sin(\phi) \dot{K}'(0)) \cdot (\cos(\phi) \nabla \nu(K(0))^T \dot{K}(0) - \sin(\phi) \nabla \nu(K'(0))^T \dot{K}'(0)) \right) \\
&\quad / (1 - \sin(2\phi) \dot{K}(0) \cdot \dot{K}'(0))^2 .
\end{aligned} \tag{3.85}$$

We can treat the singular part of the integrand in eq. (3.81) by changing to polar coordinates and replacing it with the following C^0 function (which includes the Jacobian of transformation 'r'):

$$G(r, \phi) = \begin{cases} r \times (K(r \cos(\phi)) - K'(r \sin(\phi))) \cdot \hat{\mathbf{n}}(K'(r \sin(\phi))) \\ \quad \times \frac{(K(r \cos(\phi)) - K'(r \sin(\phi))) \cdot (\nu(K(r \cos(\phi))) - \nu(K'(r \sin(\phi))))}{\|K(r \cos(\phi)) - K'(r \sin(\phi))\|^4} & r > 0 \\ (\cos(\phi) \dot{K}(0) - \sin(\phi) \dot{K}'(0)) \cdot \hat{\mathbf{n}}(K'(0)) \\ \quad \times \left((\cos(\phi) \dot{K}(0) - \sin(\phi) \dot{K}'(0)) \cdot (\cos(\phi) \nabla \nu(K(0))^T \dot{K}(0) - \sin(\phi) \nabla \nu(K'(0))^T \dot{K}'(0)) \right) \\ \quad / (1 - \sin(2\phi) \dot{K}(0) \cdot \dot{K}'(0))^2 & r = 0 . \end{cases} \tag{3.86}$$

After the transformations described above, we get the local integral in the following form:

$$\int_{\phi=0}^{\arctan(\frac{|\pi'|}{|\pi|})} \int_{r=0}^{\frac{|\pi|}{\cos(\phi)}} \mathcal{Z}(r, \phi) G(r, \phi) dr d\phi + \int_{\phi=\arctan(\frac{|\pi'|}{|\pi|})}^{\frac{\pi}{2}} \int_{r=0}^{\frac{|\pi'|}{\sin(\phi)}} \mathcal{Z}(r, \phi) G(r, \phi) dr d\phi . \tag{3.87}$$

This can be integrated as both $\mathcal{Z}(r, \phi)$ and $G(r, \phi)$ are continuous.

3.2.6 Evaluating T_V and T_{VI} in the 2D shape gradient formula

For evaluating the fifth and sixth terms in the eq. (3.15), we combine the two due to the similarities appearing in the integrand. The combined expression is given as:

$$\begin{aligned}
&= -\frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) (g(\hat{y}) \nabla \cdot \nu(\hat{y}) + \nabla g(\hat{y}) \cdot \nu(\hat{y})) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= -\frac{1}{2\pi} \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) .
\end{aligned} \tag{3.88}$$

Plugging in the value of $p(\hat{x})$, we get:

$$\begin{aligned}
&= -\frac{1}{2\pi} \sum_{i=1}^N b_i \int_{\Gamma_0} \int_{\Gamma_0} \beta_i^N(\hat{x}) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
&= -\frac{1}{2\pi} \sum_{i=1}^N b_i U_i, \\
U_i &= \int_{\Gamma_0} \int_{\Gamma_0} \beta_i^N(\hat{x}) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) .
\end{aligned} \tag{3.89}$$

Assuming the support for the basis function β_i^N is the panel π , we get:

$$\begin{aligned} U_i &= \int_{\Gamma_0} \int_{\pi} \beta_i^N(\hat{x}) \nabla \cdot (g(\hat{y})\nu(\hat{y})) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x})d\Gamma_0(\hat{y}) \\ &= \sum_{\pi' \in \mathcal{M}} \int_{\pi'} \int_{\pi} \beta_i^N(\hat{x}) \nabla \cdot (g(\hat{y})\nu(\hat{y})) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x})d\Gamma_0(\hat{y}) . \end{aligned} \quad (3.90)$$

The integrals to be evaluated are:

$$\begin{aligned} &= \int_{\pi'} \int_{\pi} \beta_i^N(\hat{x}) \nabla \cdot (g(\hat{y})\nu(\hat{y})) \frac{\hat{x} - \hat{y}}{\|\hat{x} - \hat{y}\|^2} \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x})d\Gamma_0(\hat{y}) \\ &= \int_{t=-1}^1 \int_{s=-1}^1 \hat{\beta}_k(s) \nabla \cdot (g(\gamma_{\pi'}(t))\nu(\gamma_{\pi'}(t))) \frac{\gamma_{\pi}(s) - \gamma_{\pi'}(t)}{\|\gamma_{\pi}(s) - \gamma_{\pi'}(t)\|^2} \cdot \hat{\mathbf{n}}(\gamma_{\pi'}(t)) \|\dot{\gamma}_{\pi}(s)\| \|\dot{\gamma}_{\pi'}(t)\| ds dt . \end{aligned} \quad (3.91)$$

By evaluating the local integral above for all combinations of π , π' and $\hat{\beta}_k$, and using the local to global map, we can evaluate the vector U . If $\pi \cap \pi' = \{\phi\}$, we are away from the singularity and can evaluate the integral by simply using tensor product quadrature rule.

Coinciding panels: For $\pi = \pi'$, the local integral becomes:

$$= \int_{t=-1}^1 \int_{s=-1}^1 \hat{\beta}_k(s) \nabla \cdot (g(\gamma_{\pi}(t))\nu(\gamma_{\pi}(t))) \frac{\gamma_{\pi}(s) - \gamma_{\pi}(t)}{\|\gamma_{\pi}(s) - \gamma_{\pi}(t)\|^2} \cdot \hat{\mathbf{n}}(\gamma_{\pi}(t)) \|\dot{\gamma}_{\pi}(s)\| \|\dot{\gamma}_{\pi}(t)\| ds dt . \quad (3.92)$$

The singular term in the integrand above is a Double Layer singularity. Thus it can be treated by replacing the singular term with the following C^0 function:

$$N(s, t) = \begin{cases} \frac{\gamma_{\pi}(s) - \gamma_{\pi}(t)}{\|\gamma_{\pi}(s) - \gamma_{\pi}(t)\|^2} \cdot \hat{\mathbf{n}}(\gamma_{\pi}(t)) & s \neq t \\ \frac{\dot{\gamma}_{\pi}(t) \cdot \hat{\mathbf{n}}(\gamma_{\pi}(t))}{2\|\dot{\gamma}_{\pi}(t)\|^2} & s = t . \end{cases} \quad (3.93)$$

Since the remaining integrand is also continuous, we can evaluate it by tensor product quadrature rule.

Adjacent panels: For the case of adjacent panels or $\pi \cap \pi' = \{P\}$, we transform the local integral into arclength coordinates by using the coordinate transformations mentioned in eq. (3.59). Renaming s' and t' to s and t respectively, we get:

$$\begin{aligned} &= \frac{4}{|\pi||\pi'|} \int_{t=0}^{|\pi'|} \int_{s=0}^{|\pi|} \frac{(K(s) - K'(t)) \cdot \hat{\mathbf{n}}(K'(t))}{\|K(s) - K'(t)\|^2} \nabla \cdot (g(K'(t))\nu(K'(t))) \\ &\quad \hat{\beta}_k(1 - \frac{2s}{|\pi|}) \|\dot{\gamma}_{\pi}(1 - \frac{2s}{|\pi|})\| \|\dot{\gamma}_{\pi'}(\frac{2t}{|\pi'|} - 1)\| ds dt . \end{aligned} \quad (3.94)$$

To treat the singular term, we use Taylor expansion and switch to polar coordinates. This is already done in eq. (3.83). So we can simply replace the singular term by the following C^0 function (which includes the Jacobian of transformation r):

$$B(r, \phi) = \begin{cases} r \times \frac{(K(r \cos(\phi)) - K'(r \sin(\phi))) \cdot \hat{\mathbf{n}}(K'(r \sin(\phi)))}{\|K(r \cos(\phi)) - K'(r \sin(\phi))\|^2} & r \neq 0 \\ \frac{(\cos(\phi)\dot{K}(0) - \sin(\phi)\dot{K}'(0)) \cdot \hat{\mathbf{n}}(K'(0))}{1 - \sin(2\phi)\dot{K}(0) \cdot \dot{K}'(0)} & r = 0 . \end{cases} \quad (3.95)$$

Using the transformations, the local integral has the following form:

$$\int_{\phi=0}^{\arctan(\frac{|\pi'|}{|\pi|})} \int_{r=0}^{\frac{|\pi|}{\cos(\phi)}} \mathcal{Z}(r, \phi) B(r, \phi) dr d\phi + \int_{\phi=\arctan(\frac{|\pi'|}{|\pi|})}^{\frac{\pi}{2}} \int_{r=0}^{\frac{|\pi'|}{\sin(\phi)}} \mathcal{Z}(r, \phi) B(r, \phi) dr d\phi . \quad (3.96)$$

With $\mathcal{Z}(r, \phi)$ and $B(r, \phi)$ being continuous, we can evaluate the integral by tensor product quadrature rule.

3.3 Stable Evaluation

When numerically evaluating the expressions above which are singular but have a finite limit, we need to take care of cancellation errors as mentioned in the notes [3, Ch. 1, Sec. 1.5.43]. The cancellation error occurs when two almost same quantities are subtracted. The original numbers are already inexact when stored on the machine. Subtracting two close numbers stored on the machine may lead to a large relative error which is undesirable. This is demonstrated in the figure 1 where the white and red bars denote the true values and absolute errors respectively. Notice that after subtraction, the size of the absolute error (red) is comparable to the size of the true value (white) which means a very high relative error.

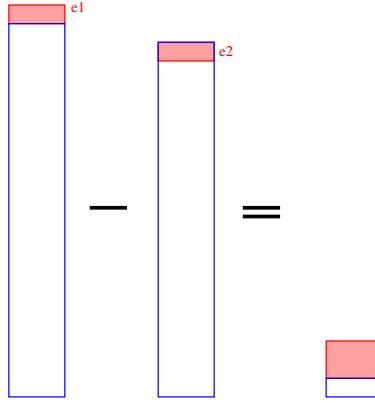


Figure 1: Cancellation error

For evaluating the derived expressions in the previous sub-section, we can simply look at two cases: coinciding panels and adjacent panels. When we have coinciding panels, we encounter expressions of the form:

$$\frac{f(s) - f(t)}{s - t}. \quad (3.97)$$

For $s \rightarrow t$, we have the limit $\dot{f}(t)$ for the expression above. Question is when evaluating it numerically, when to use the this limit and when to evaluate the difference quotient. As mentioned above, the numbers stored on the machine are approximations of the true number. When storing a number whose true value is 'a', what's stored on the machine is something like:

$$a(1 + \delta), \quad |\delta| < \epsilon_m. \quad (3.98)$$

ϵ_m is the machine epsilon. Using this representation, the difference quotient becomes:

$$\begin{aligned} &= \frac{f(s)(1 + \delta_1) - f(t)(1 + \delta_2)}{s - t}, \quad |\delta_1|, |\delta_2| < \epsilon_m \\ &= \frac{f(t+h)(1 + \delta_1) - f(t)(1 + \delta_2)}{h} \\ &= \frac{f(t+h) - f(t)}{h} + \frac{\delta_1 f(t+h) - \delta_2 f(t)}{h}. \end{aligned} \quad (3.99)$$

The first term is the actual difference quotient, the second term is the error. For $h \rightarrow 0$, the error is:

$$\left| \frac{\delta_1 f(t) - \delta_2 f(t)}{h} \right| \leq \frac{|\delta_1 f(t)|}{h} + \frac{|\delta_2 f(t)|}{h} \leq \frac{2\epsilon_m |f(t)|}{h} = O(h^{-1}). \quad (3.100)$$

When we use the Taylor series approximation:

$$f(s) = f(t) + (s - t)\dot{f}(t) + \frac{(s - t)^2}{2}\ddot{f}(t) + \dots, \quad (3.101)$$

The error that we incur from approximating the difference quotient by the first derivative:

$$\frac{f(s) - f(t)}{s - t} - \dot{f}(t) = \frac{(s - t)}{2} \ddot{f}(t) + O((s - t)^2) = O(h). \quad (3.102)$$

To choose the split point where we switch to the Taylor approximation can be calculated by simply equating the two errors.

$$\begin{aligned} \frac{h}{2} |\ddot{f}(t)| &= \frac{2\epsilon_m |f(t)|}{h} \\ \implies h &= 2\sqrt{\epsilon_m} \sqrt{\left| \frac{f(t)}{\ddot{f}(t)} \right|} = O(\sqrt{\epsilon_m}). \end{aligned} \quad (3.103)$$

For evaluating the difference coefficient, we simply evaluate it when $|s - t| \geq \sqrt{\epsilon_m}$ and use the Taylor approximation otherwise:

$$\frac{f(s) - f(t)}{s - t} \approx \dot{f}\left(\frac{s + t}{2}\right), \quad |s - t| < \sqrt{\epsilon_m}. \quad (3.104)$$

The same idea applies in the expressions emerging in the adjacent panels case. There instead of $|s - t|$, we have r . For $r > \sqrt{\epsilon_m}$ we simply evaluate the expression, otherwise the Taylor approximation is used.

4 Energy shape gradient using variational formulation for the Laplacian

In this section, we derive the shape gradient of the energy functional but using a variational formulation for the Laplacian equation instead of the direct first kind BEM formulation. We do this because we cannot directly compare the shape gradient formula and the total force formula obtained using the Maxwell stress tensor. Instead we find another shape gradient formula which carries the same issues as in the total force formula. Such a comparison of different shape gradient formulas is also done by Paganini and Hiptmair [7] where they compare volume and boundary based shape gradient formulas, which although equivalent on a smooth level, show differences in numerical evaluation.

4.1 Volume Formula using Lagrangian Pullback Approach

In this section, we derive a volume based shape gradient formula for the energy functional using the Lagrangian pullback approach, starting from the natural variational formulation for the Laplace equation.

$$\Delta u = 0 \text{ in } \Omega, \quad u = g \text{ on } \partial\Omega \quad (4.1)$$

Multiplying with a test function v and integrating over the domain,

$$\int_{\Omega} \Delta u v \, dx = 0, \quad u \in H^1(\Omega), \forall v \in H_0^1(\Omega). \quad (4.2)$$

Using Green's identity we get:

$$\int_{\Omega} \nabla u \cdot \nabla v \, dx = 0. \quad (4.3)$$

The energy functional in volume representation, as given in eq. (2.5):

$$= \frac{1}{2} \int_{\Omega} |\nabla u|^2 \, dx. \quad (4.4)$$

Since u and v are in different spaces, we use the offset function technique

$$u = \tilde{u} + f, \quad \tilde{u} \in H_0^1(\Omega), \quad f \in H^1(\Omega), \quad f|_{\partial\Omega} = g. \quad (4.5)$$

Using the offset function technique, we get the variational formulation:

$$a(\tilde{u}, v) = l(v), \quad a(\tilde{u}, v) := \int_{\Omega} \nabla \tilde{u} \cdot \nabla v \, dx, \quad l(v) := - \int_{\Omega} \nabla f \cdot \nabla v \, dx. \quad (4.6)$$

For convenience, we use the symbol u instead of \tilde{u}

$$a(u, v) = l(v), \quad a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad l(v) = - \int_{\Omega} \nabla f \cdot \nabla v \, dx. \quad (4.7)$$

The energy functional, using eq. (4.5) and writing u instead of \tilde{u} :

$$J(\Omega, u) = \frac{1}{2} \int_{\Omega} |\nabla u + \nabla f|^2 \, dx. \quad (4.8)$$

Using the same perturbation method as in derivation for direct first kind formulation, we get the 't' dependent integrals:

$$\begin{aligned} J(t, u) &= \frac{1}{2} \int_{\Omega_t} |\nabla u(x) + \nabla f(x)|^2 \, dx, \quad u \in H_0^1(\Omega_t) \\ &= \frac{1}{2} \int_{\Omega_0} |DT_t^{-T} \hat{\nabla}(u(T_t(\hat{x}))) + G(T_t(\hat{x}))|^2 J_t(\hat{x}) \, d\hat{x}, \quad G := \nabla f. \\ a(t, u, v) &= \int_{\Omega_t} \nabla u(x) \cdot \nabla v(x) \, dx, \quad u \in H_0^1(\Omega_t), \quad \forall v \in H_0^1(\Omega_t) \\ &= \int_{\Omega_0} DT_t^{-T} \hat{\nabla} u(T_t(\hat{x})) \cdot DT_t^{-T} \hat{\nabla} v(T_t(\hat{x})) J_t(\hat{x}) \, d\hat{x}. \\ l(t, v) &= - \int_{\Omega_t} G(x) \cdot \nabla v(x) \, dx, \quad \forall v \in H_0^1(\Omega_t) \\ &= - \int_{\Omega_0} G(T_t(\hat{x})) \cdot DT_t^{-T} \hat{\nabla} v(T_t(\hat{x})) J_t(\hat{x}) \, d\hat{x}. \end{aligned} \quad (4.9)$$

The above expressions are obtained using the following identities:

$$\begin{aligned} \int_{\Omega_t} f(x) \, dx &= \int_{\Omega_0} f(T_t(\hat{x})) J_t(\hat{x}) \, d\hat{x}, \\ \hat{\nabla}(F(T_t(\hat{x}))) &= \hat{D}T_t^T(\hat{x})(\nabla F)(T_t(\hat{x})). \end{aligned} \quad (4.10)$$

In the transformations above, ∇g is not transformed using the gradient transformation formula as it is a known function in volume which is independent of these shape transformations. Using the pullback from eq. (2.20) we get:

$$\begin{aligned} J(t, u) &= \hat{J}(t, \hat{u}) = \frac{1}{2} \int_{\Omega_0} |DT_t^{-T}(\hat{x}) \hat{\nabla}(\hat{u}(\hat{x})) + G(T_t(\hat{x}))|^2 J_t(\hat{x}) \, d\hat{x}, \\ \hat{a}(t, \hat{u}, \hat{v}) &= a(t, u, v) = \int_{\Omega_0} DT_t^{-T}(\hat{x}) \hat{\nabla} \hat{u}(\hat{x}) \cdot DT_t^{-T}(\hat{x}) \hat{\nabla} \hat{v}(\hat{x}) J_t(\hat{x}) \, d\hat{x}, \quad \hat{u}, \hat{v} \in H_0^1(\Omega_0), \\ \hat{l}(t, \hat{v}) &= l(t, v) = - \int_{\Omega_0} G(T_t(\hat{x})) \cdot DT_t^{-T}(\hat{x}) \hat{\nabla} \hat{v}(\hat{x}) J_t(\hat{x}) \, d\hat{x}. \end{aligned} \quad (4.11)$$

The Lagrangian is defined as:

$$L(t, \hat{u}, \hat{v}) := \hat{J}(t, \hat{u}) + \hat{a}(t, \hat{u}, \hat{v}) - \hat{l}(t, \hat{v}), \quad \hat{u}, \hat{v} \in H_0^1(\Omega_0). \quad (4.12)$$

Replacing \hat{u} by \hat{u}_t , the state solution, such that:

$$\hat{a}(t, \hat{u}_t, \hat{v}) = \hat{l}(t, \hat{v}), \quad \forall \hat{v} \in H_0^1(\Omega_0), \quad (4.13)$$

the lagrangian becomes:

$$L(t, \hat{u}_t, \hat{v}) = \hat{J}(t, \hat{u}_t) = \mathcal{J}(t) \quad (4.14)$$

The shape gradient is given as:

$$= \frac{d(\mathcal{J}(t))}{dt} \Big|_{t=0} = \frac{\partial L(t, \hat{u}_t, \hat{v})}{\partial t} \Big|_{t=0} + \frac{\partial L(t, \hat{u}_t, \hat{v}; \frac{d\hat{u}_t}{dt})}{\partial \hat{u}} \Big|_{t=0}. \quad (4.15)$$

In the expression above, putting the second term equal to zero gives the adjoint equation.

$$\begin{aligned} &= \frac{\partial L(t, \hat{u}_t, \hat{v}; \eta)}{\partial \hat{u}} \Big|_{t=0} = \frac{\partial \hat{J}(t, \hat{u}_t; \eta)}{\partial \hat{u}} \Big|_{t=0} + \frac{\partial \hat{a}(t, \hat{u}_t, \hat{v}; \eta)}{\partial \hat{u}} \Big|_{t=0}, \quad \forall \eta \in H_0^1(\Omega_0) \\ &= \frac{1}{2} \int_{\Omega_0} \det(DT_t(\hat{x})) \left[2(DT_t^{-T}(\hat{x}) \hat{\nabla}(\hat{u}_t) + G(T_t(\hat{x}))) \cdot (DT_t^{-T}(\hat{x}) \hat{\nabla} \eta(\hat{x})) \right] d\hat{x} \\ &\quad + \int_{\Omega_0} DT_t^{-T}(\hat{x}) \hat{\nabla} \eta(\hat{x}) \cdot DT_t^{-T}(\hat{x}) \hat{\nabla} \hat{v}(\hat{x}) \det(DT_t(\hat{x})) d\hat{x}. \end{aligned}$$

At $t = 0$:

$$= \int_{\Omega_0} (\hat{\nabla}(u_0(\hat{x}) + f(\hat{x})) \cdot \hat{\nabla} \eta(\hat{x})) d\hat{x} + \int_{\Omega_0} \hat{\nabla} \eta(\hat{x}) \cdot \hat{\nabla} \hat{v}(\hat{x}) d\hat{x}. \quad (4.16)$$

The first term in the expression above is zero as it is the state equation for Ω_0 . This implies that the adjoint solution \hat{v} is trivial. We get the shape gradient by partial derivative of the Lagrangian:

$$\begin{aligned} \frac{d(\mathcal{J}(t))}{dt} \Big|_{t=0} &= \frac{\partial L(t, \hat{u}_t, \hat{v})}{\partial t} \Big|_{t=0} = \frac{\partial \hat{J}(t, \hat{u}_t)}{\partial t} \Big|_{t=0} + \frac{\partial \hat{a}(t, \hat{u}_t, \hat{v})}{\partial t} \Big|_{t=0} + \frac{\partial \hat{l}(t, \hat{v})}{\partial t} \Big|_{t=0} \\ &= \frac{\partial \hat{J}(t, \hat{u}_t)}{\partial t} \Big|_{t=0}, \quad \hat{v} = 0 \\ &= \frac{1}{2} \int_{\Omega_0} \left\{ |DT_t^{-T}(\hat{x}) \hat{\nabla}(\hat{u}_t(\hat{x})) + G(T_t(\hat{x}))|^2 \hat{\nabla} \cdot \nu(\hat{x}) + 2 \det(DT_t(\hat{x})) \right. \\ &\quad \left. (DT_t^{-T}(\hat{x}) \hat{\nabla} \hat{u}_t(\hat{x}) + G(T_t(\hat{x}))) \cdot \left(-\hat{\nabla} \nu(\hat{x}) \hat{\nabla} \hat{u}_t(\hat{x}) + (\nabla G)(T_t(\hat{x}))^T \nu(\hat{x}) \right) \right\} d\hat{x}. \end{aligned}$$

At $t = 0$:

$$\begin{aligned} &= \frac{1}{2} \int_{\Omega_0} \left(|\hat{\nabla}(u_0(\hat{x}) + f(\hat{x}))|^2 \hat{\nabla} \cdot \nu(\hat{x}) + 2(\hat{\nabla}(u_0(\hat{x}) + f(\hat{x}))) \cdot \left(-\hat{\nabla} \nu(\hat{x}) \hat{\nabla} u_0(\hat{x}) + \hat{\nabla} \hat{\nabla} f(\hat{x})^T \nu(\hat{x}) \right) \right) d\hat{x} \\ &= \frac{1}{2} \int_{\Omega_0} \left(|\hat{\nabla} u(\hat{x})|^2 \hat{\nabla} \cdot \nu(\hat{x}) + 2(\hat{\nabla} u(\hat{x})) \cdot \left(-\hat{\nabla} \nu(\hat{x}) \hat{\nabla} u(\hat{x}) + \hat{\nabla} \nu(\hat{x}) \hat{\nabla} f(\hat{x}) + \hat{\nabla} \hat{\nabla} f(\hat{x})^T \nu(\hat{x}) \right) \right) d\hat{x}. \end{aligned} \quad (4.17)$$

Theorem 4.1. *The volume based shape gradient formula for the energy functional in eq. (2.5), with the variational constraint in eq. (4.3) is given as:*

$$= \frac{1}{2} \int_{\Omega_0} \left(|\hat{\nabla} u(\hat{x})|^2 \hat{\nabla} \cdot \nu(\hat{x}) + 2(\hat{\nabla} u(\hat{x})) \cdot \left(-\hat{\nabla} \nu(\hat{x}) \hat{\nabla} u(\hat{x}) + \hat{\nabla} \nu(\hat{x}) \hat{\nabla} f(\hat{x}) + \hat{\nabla} \hat{\nabla} f(\hat{x})^T \nu(\hat{x}) \right) \right) d\hat{x}. \quad (4.18)$$

4.2 Boundary Formula Using variational formulation for the Laplacian

For this derivation, we will use a variational formulation where the spaces are independent of Ω [8, Ch1. 2, eq. 2.14]. For the Dirichlet problem, we seek $u \in H^1(D)$, $\mu \in H(\text{div } 0, D)$:

$$\begin{aligned} \int_{\Omega} \nabla u \cdot \nabla v dx + \int_{\partial \Omega} v \mu \cdot n dS &= 0, \quad \forall v \in H^1(D), \\ \int_{\partial \Omega} u \lambda \cdot n dS &= \int_{\partial \Omega} g \lambda \cdot n dS, \quad \forall \mu \in H(\text{div } 0, D). \end{aligned}$$

The variational formulation above can be written as:

$$\begin{aligned}
a(\Omega, (u, \mu), (v, \lambda)) &= l(\Omega, (v, \lambda)), \\
a(\Omega, (u, \mu), (v, \lambda)) &:= \int_{\Omega} \nabla u \cdot \nabla v \, dx + \int_{\partial\Omega} v \, \mu \cdot n \, dS + \int_{\partial\Omega} u \, \lambda \cdot n \, dS, \\
l(\Omega, (v, \lambda)) &:= \int_{\partial\Omega} g \, \lambda \cdot n \, dS.
\end{aligned} \tag{4.19}$$

The energy functional is given as:

$$J(\Omega, u) = \frac{1}{2} \int_{\Omega} |\nabla u|^2 \, dx = \frac{1}{2} a(\Omega, (u, 0), (u, 0)). \tag{4.20}$$

Now we define the Lagrangian as follows:

$$\begin{aligned}
\mathcal{L}(\Omega, (u, \mu), (v, \lambda)) &:= J(\Omega, u) + a(\Omega, (u, \mu), (v, \lambda)) - l(\Omega, (v, \lambda)) \\
&= a(\Omega, (u, 0), (u, 0)) + a(\Omega, (u, \mu), (v, \lambda)) - l(\Omega, (v, \lambda)).
\end{aligned} \tag{4.21}$$

When $u = u(\Omega)$ and $\mu = \mu(\Omega)$:

$$\begin{aligned}
&a(\Omega, (u(\Omega), \mu(\Omega)), (v, \lambda)) - l(\Omega, (v, \lambda)) = 0 \\
\implies \mathcal{L}(\Omega, (u(\Omega), \mu(\Omega)), (v, \lambda)) &= J(\Omega, u(\Omega)) = \mathcal{J}(\Omega).
\end{aligned} \tag{4.22}$$

The shape gradient is given as:

$$\left\langle \frac{d\mathcal{J}(\Omega)}{d\Omega}; \nu \right\rangle = \left\langle \frac{\partial \mathcal{L}(\Omega, (u(\Omega), \mu(\Omega)), (p, \Pi))}{\partial \Omega}; \nu \right\rangle. \tag{4.23}$$

p and Π are the solutions of the adjoint problem which is given as:

$$\begin{aligned}
&\left\langle \frac{\partial \mathcal{L}(\Omega, X(\Omega), (p, \Pi))}{\partial X}; \eta \right\rangle = 0, \quad \forall \eta \in H^1(D) \times H(\operatorname{div} 0, D) \\
\implies \left\langle \frac{\partial J(\Omega, u(\Omega))}{\partial u}; v \right\rangle + \left\langle \frac{\partial a(\Omega, X(\Omega), (p, \Pi))}{\partial X}; \eta \right\rangle &= 0.
\end{aligned}$$

In the equations above $X := (u, \mu)$ and $\eta := (v, \lambda)$. On simplifying we get:

$$\begin{aligned}
a(\Omega, (v, \lambda), (p, \Pi)) &= - \int_{\Omega} \nabla u(\Omega) \cdot \nabla v \, dx \\
\int_{\Omega} \nabla p \cdot \nabla v \, dx + \int_{\partial\Omega} v \, \Pi \cdot n \, dS + \int_{\partial\Omega} p \, \lambda \cdot n \, dS &= - \int_{\Omega} \nabla u(\Omega) \cdot \nabla v \, dx \\
&= - \int_{\partial\Omega} \nabla u(\Omega) \cdot n \, v \, dS.
\end{aligned}$$

The last step in the equation above uses the Green's identity. We can solve for p and Π :

$$\begin{aligned}
\int_{\partial\Omega} p \, \lambda \cdot n \, dS = 0 \quad \forall \lambda &\implies p = 0, \\
\int_{\partial\Omega} v \, \Pi \cdot n \, dS = - \int_{\partial\Omega} \nabla u(\Omega) \cdot n \, v \, dS &\implies \Pi = - \nabla u(\Omega).
\end{aligned}$$

Now we calculate the partial derivative of the Lagrangian with respect to Ω to get the shape gradient. For that, we use this simple identity for shape gradient of an integral with the integrand independent of the shape [1, Ch. 9, Thm 4.1]:

$$\begin{aligned}
I(\Omega) &= \int_{\Omega} f(x) \, dx, \\
\left\langle \frac{dI(\Omega)}{d\Omega}; \nu \right\rangle &= \int_{\partial\Omega} f(x) \, \nu(x) \cdot n(x) \, dS.
\end{aligned} \tag{4.24}$$

Using the definition of the Lagrangian we get:

$$\begin{aligned} & \left\langle \frac{\partial \mathcal{L}(\Omega, (u(\Omega), \mu(\Omega)), (p, \Pi))}{\partial \Omega}; \nu \right\rangle = \\ & \left\langle \frac{\partial J(\Omega, u(\Omega))}{\partial \Omega}; \nu \right\rangle + \left\langle \frac{\partial a(\Omega, (u(\Omega), \mu(\Omega)), (p, \Pi))}{\partial \Omega}; \nu \right\rangle - \left\langle \frac{\partial l(\Omega, (p, \Pi))}{\partial \Omega}; \nu \right\rangle . \end{aligned} \quad (4.25)$$

Now we calculate the shape gradient for individual terms. For J , we directly get:

$$\left\langle \frac{\partial J(\Omega, u(\Omega))}{\partial \Omega}; \nu \right\rangle = \frac{1}{2} \int_{\partial \Omega} |\nabla u(\Omega)|^2 \nu \cdot n \, dS . \quad (4.26)$$

For a we calculate it as follows:

$$\begin{aligned} a(\Omega, (u(\Omega), \mu(\Omega)), (0, -\nabla u(\Omega))) &= - \int_{\partial \Omega} u(\Omega) \nabla u(\Omega) \cdot n \, dS \\ &= - \int_{\Omega} \nabla \cdot (u(\Omega) \nabla u(\Omega)) \, dx \quad (\text{Divergence Theorem}) \\ &= - \int_{\Omega} |\nabla u(\Omega)|^2 \, dx, \quad \nabla \cdot \nabla u(\Omega) = 0 \\ \implies \left\langle \frac{\partial a(\Omega, (u(\Omega), \mu(\Omega)), (p, \Pi))}{\partial \Omega}; \nu \right\rangle &= - \int_{\partial \Omega} |\nabla u(\Omega)|^2 \nu \cdot n \, dS . \end{aligned} \quad (4.27)$$

For l we calculate it as follows:

$$\begin{aligned} l(\Omega, (0, -\nabla u(\Omega))) &= - \int_{\partial \Omega} g \nabla u(\Omega) \cdot n \, dS = - \int_{\Omega} \nabla g \cdot \nabla u(\Omega) \, dx \\ \implies \left\langle \frac{\partial l(\Omega, (p, \Pi))}{\partial \Omega}; \nu \right\rangle &= - \int_{\partial \Omega} \nabla g \cdot \nabla u(\Omega) \nu \cdot n \, dx . \end{aligned} \quad (4.28)$$

Adding the individual terms, we get the final shape gradient:

$$\begin{aligned} &= \frac{1}{2} \int_{\partial \Omega} |\nabla u(\Omega)|^2 \nu \cdot n \, dS - \int_{\partial \Omega} |\nabla u(\Omega)|^2 \nu \cdot n \, dS + \int_{\partial \Omega} \nabla g \cdot \nabla u(\Omega) \nu \cdot n \, dx \\ &= \frac{1}{2} \int_{\partial \Omega} (\nabla g - \nabla u(\Omega)) \cdot \nabla u(\Omega) \nu \cdot n \, dS + \frac{1}{2} \int_{\partial \Omega} \nabla g \cdot \nabla u(\Omega) \nu \cdot n \, dx . \end{aligned} \quad (4.29)$$

Note that $g = \nabla u$ on the boundary $\partial \Omega$ so $\nabla g - \nabla u$ is entirely in the normal direction. Thus the formula above becomes:

Theorem 4.2. *The boundary based shape gradient formula for the energy functional in eq. (2.5), with the variational constraint in eq. (4.3) is given as:*

$$= \frac{1}{2} \int_{\partial \Omega} ((\nabla g - \nabla u(\Omega)) \cdot n) (\nabla u(\Omega) \cdot n) \nu \cdot n \, dS + \frac{1}{2} \int_{\partial \Omega} \nabla g \cdot \nabla u(\Omega) \nu \cdot n \, dx .$$

4.3 Boundary Formula Using Mixed Variational Formulation

In this section we try to derive the boundary formula, as in the previous sub-section, but using the mixed variational formulation for the Dirichlet BVP [6, Sec. 6]. We seek $u \in L^2(D)$ and $\vec{q} \in H(\text{div}; D)$ such that:

$$\begin{aligned} \int_{\Omega} \vec{q} \cdot \vec{p} \, dx + \int_{\Omega} u \nabla \cdot \vec{p} \, dx &= \int_{\partial \Omega} g \vec{p} \cdot n \, dx, \quad \forall \vec{p} \in H(\text{div}; D), \quad \vec{q} := \nabla u, \\ \int_{\Omega} \nabla \cdot \vec{q} \, v \, dx &= 0, \quad \forall v \in L^2(D) . \end{aligned} \quad (4.30)$$

The variational formulation above can be written as:

$$\begin{aligned}
a(\Omega, (u, \vec{q}), (v, \vec{p})) &= l(\Omega, (v, \vec{p})), \\
a(\Omega, (u, \vec{q}), (v, \vec{p})) &:= \int_{\Omega} \vec{q} \cdot \vec{p} \, dx + \int_{\Omega} u \nabla \cdot \vec{p} \, dx + \int_{\Omega} \nabla \cdot \vec{q} v \, dx . \\
l(\Omega, (v, \vec{p})) &:= \int_{\partial\Omega} g \vec{p} \cdot n \, dx .
\end{aligned} \tag{4.31}$$

The energy functional is given as:

$$J(\Omega, \vec{q}) = \frac{1}{2} \int_{\Omega} |\vec{q}|^2 \, dx . \tag{4.32}$$

The Lagrangian is defined as:

$$\mathcal{L}(\Omega, (u, \vec{q}), (v, \vec{p})) := J(\Omega, \vec{q}) + a(\Omega, (u, \vec{q}), (v, \vec{p})) - l(\Omega, (v, \vec{p})) . \tag{4.33}$$

Putting in the state solution $(u(\Omega), \vec{q}(\Omega))$, we get:

$$\mathcal{L}(\Omega, (u(\Omega), \vec{q}(\Omega)), (v, \vec{p})) = J(\Omega, \vec{q}(\Omega)) = \mathcal{J}(\Omega) . \tag{4.34}$$

The shape gradient is given as:

$$\left\langle \frac{d\mathcal{J}(\Omega)}{d\Omega}; \nu \right\rangle = \left\langle \frac{\partial \mathcal{L}(\Omega, (u(\Omega), \vec{q}(\Omega)), (w, \vec{r}))}{\partial \Omega}; \nu \right\rangle . \tag{4.35}$$

Where $(w, \vec{r}) \in L^2(D) \times H(\text{div}; D)$ solve the adjoint problem:

$$\begin{aligned}
&\left\langle \frac{\partial \mathcal{L}(\Omega, X(\Omega), (w, \vec{r}))}{\partial X}; \eta \right\rangle = 0, \quad \forall \eta \in L^2(D) \times H(\text{div}; D) . \\
\implies &\left\langle \frac{\partial J(\Omega, \vec{q}(\Omega))}{\partial \vec{q}}; \vec{p} \right\rangle + \left\langle \frac{\partial a(\Omega, X(\Omega), (w, \vec{r}))}{\partial X}; \eta \right\rangle = 0,
\end{aligned} \tag{4.36}$$

where $X := (u, \vec{q})$ and $\eta := (v, \vec{p})$. Simplifying above expression we get:

$$\begin{aligned}
a(\Omega, (v, \vec{p}), (w, \vec{r})) &= - \int_{\Omega} \vec{q}(\Omega) \cdot \vec{p} \, dx \\
\int_{\Omega} \vec{p} \cdot \vec{r} \, dx + \int_{\Omega} v \nabla \cdot \vec{r} \, dx + \int_{\Omega} w \nabla \cdot \vec{p} \, dx &= - \int_{\Omega} \vec{q}(\Omega) \cdot \vec{p} \, dx .
\end{aligned} \tag{4.37}$$

The adjoint solution (w, \vec{r}) can be found as:

$$\begin{aligned}
\int_{\Omega} v \nabla \cdot \vec{r} \, dx &= 0 \quad \forall v \implies \nabla \cdot \vec{r} = 0, \\
\int_{\Omega} \vec{p} \cdot \vec{r} \, dx + \int_{\Omega} w \nabla \cdot \vec{p} \, dx &= - \int_{\Omega} \vec{q}(\Omega) \cdot \vec{p} \, dx \implies \vec{r} = - \nabla u(\Omega), \quad w = 0 .
\end{aligned} \tag{4.38}$$

We use the shape gradient formula for integrals from eq. (4.24). Using the definition of Lagrangian we get:

$$\begin{aligned}
&\left\langle \frac{\partial \mathcal{L}(\Omega, (u(\Omega), \vec{q}(\Omega)), (w, \vec{r}))}{\partial \Omega}; \nu \right\rangle = \\
&\left\langle \frac{\partial J(\Omega, \vec{q}(\Omega))}{\partial \Omega}; \nu \right\rangle + \left\langle \frac{\partial a(\Omega, (u(\Omega), \vec{q}(\Omega)), (w, \vec{r}))}{\partial \Omega}; \nu \right\rangle - \left\langle \frac{\partial l(\Omega, (w, \vec{r}))}{\partial \Omega}; \nu \right\rangle .
\end{aligned} \tag{4.39}$$

Now we calculate the shape gradients for individual terms. For J it is directly given as:

$$\left\langle \frac{\partial J(\Omega, \vec{q}(\Omega))}{\partial \Omega}; \nu \right\rangle = \frac{1}{2} \int_{\partial\Omega} |\vec{q}(\Omega)|^2 \nu \cdot n \, dS = \frac{1}{2} \int_{\partial\Omega} |\nabla u(\Omega)|^2 \nu \cdot n \, dS . \tag{4.40}$$

For a we calculate it as follows:

$$\begin{aligned}
a(\Omega, (u(\Omega), \vec{q}(\Omega)), (0, -\nabla u(\Omega))) &= - \int_{\Omega} \vec{q}(\Omega) \cdot \nabla u(\Omega) dS \\
&= - \int_{\Omega} |\nabla u(\Omega)|^2 dx \\
\implies \left\langle \frac{\partial a(\Omega, (u(\Omega), \vec{q}(\Omega)), (w, \vec{r}))}{\partial \Omega}; \nu \right\rangle &= - \int_{\partial \Omega} |\nabla u(\Omega)|^2 \nu \cdot n dS .
\end{aligned} \tag{4.41}$$

For l we calculate it as follows:

$$\begin{aligned}
l(\Omega, (0, -\nabla u(\Omega))) &= - \int_{\partial \Omega} g \nabla u(\Omega) \cdot n dS = - \int_{\Omega} \nabla g \cdot \nabla u(\Omega) dx \\
\implies \left\langle \frac{\partial l(\Omega, (w, \vec{r}))}{\partial \Omega}; \nu \right\rangle &= - \int_{\partial \Omega} \nabla g \cdot \nabla u(\Omega) \nu \cdot n dx .
\end{aligned} \tag{4.42}$$

Using the individual terms, we get the final shape gradient:

$$\begin{aligned}
&= \frac{1}{2} \int_{\partial \Omega} |\nabla u(\Omega)|^2 \nu \cdot n dS - \int_{\partial \Omega} |\nabla u(\Omega)|^2 \nu \cdot n dS + \int_{\partial \Omega} \nabla g \cdot \nabla u(\Omega) \nu \cdot n dx \\
&= \frac{1}{2} \int_{\partial \Omega} (\nabla g - \nabla u(\Omega)) \cdot \nabla u(\Omega) \nu \cdot n dS + \frac{1}{2} \int_{\partial \Omega} \nabla g \cdot \nabla u(\Omega) \nu \cdot n dx .
\end{aligned} \tag{4.43}$$

Note that the formula matches exactly with eq. (4.29)

4.4 Proof of equivalency of Volume and Boundary formulas

We start with the Volume formula :

$$\frac{1}{2} \int_{\Omega} \left(|\nabla u(x)|^2 \nabla \cdot \nu(x) + 2 \left(\nabla u(x) \right) \cdot \left(-\nabla \nu(x) \nabla u(x) + \nabla \nu(x) \nabla f(x) + \nabla \nabla f(x)^T \nu(x) \right) \right) dx .$$

This can be written as :

$$\begin{aligned}
&\frac{1}{2} \int_{\Omega} \left(\nabla \cdot \left(|\nabla u(x)|^2 \nu(x) \right) \right. \\
&\quad \left. + 2 \left(\nabla u(x) \right) \cdot \left(-\nabla \nu(x) \nabla u(x) + \nabla \nu(x) \nabla f(x) + \nabla \nabla f(x)^T \nu(x) - \nabla \nabla u(x)^T \nu(x) \right) \right) dx .
\end{aligned} \tag{4.44}$$

Since $\nabla \nabla u$ and $\nabla \nabla f$ are symmetric, the highlighted terms can be combined together to give:

$$\frac{1}{2} \int_{\Omega} \nabla \cdot \left(|\nabla u(x)|^2 \nu(x) \right) + 2 \left(\nabla u(x) \right) \cdot \left(-\nabla(\nu(x) \cdot \nabla u(x)) + \nabla(\nu(x) \cdot \nabla f(x)) \right) dx .$$

This can be further simplified by combining the two highlighted terms:

$$\frac{1}{2} \int_{\Omega} \nabla \cdot \left(|\nabla u(x)|^2 \nu(x) \right) + 2 \nabla u(x) \cdot \nabla \left(\nu(x) \cdot (\nabla f(x) - \nabla u(x)) \right) dx .$$

Using the Divergence theorem for the first term and Green's first formula for the second term, we get:

$$\frac{1}{2} \int_{\partial \Omega} |\nabla u(x)|^2 \nu(x) \cdot n(x) dS(x) + \int_{\partial \Omega} \nabla u(x) \cdot n(x) \left(\nu(x) \cdot (\nabla f(x) - \nabla u(x)) \right) dS(x) .$$

On the boundary, we know that $\nabla f - \nabla u$ is in the normal direction. Using that we get:

$$\frac{1}{2} \int_{\partial \Omega} |\nabla u(x)|^2 \nu(x) \cdot n(x) dS(x) + \int_{\partial \Omega} \nabla u(x) \cdot n(x) (\nabla f(x) - \nabla u(x)) \cdot n(x) \nu(x) \cdot n(x) dS(x) .$$

Whis can be rewritten as:

$$\frac{1}{2} \int_{\partial \Omega} |\nabla u(x)|^2 \nu(x) \cdot n(x) dS(x) + \int_{\partial \Omega} \nabla u(x) \cdot (\nabla f(x) - \nabla u(x)) \nu(x) \cdot n(x) dS(x) .$$

This is the boundary formula from eq. (4.29) with $f = g$

5 Numerical Experiments

The shape gradient formula was implemented using the 2D-ParametricBEM framework in C++ [9]. For evaluating both the state and adjoint solutions, and the shape gradient formulas, lowest order BEM spaces are used. Meshes used are parametric in nature (like the domains) and are uniformly spaced in the parameter domain for the parametrization. In case of annular domains where we have two different parametrizations for the two boundaries, mesh is generated by splitting the two boundaries independently with uniform spacing in the parameter domain for both. ¹

5.1 Validation of BEM shape gradient formula

For validation of the BEM shape gradient formula we restrict ourselves to smooth domains.

5.1.1 Model Problem 1

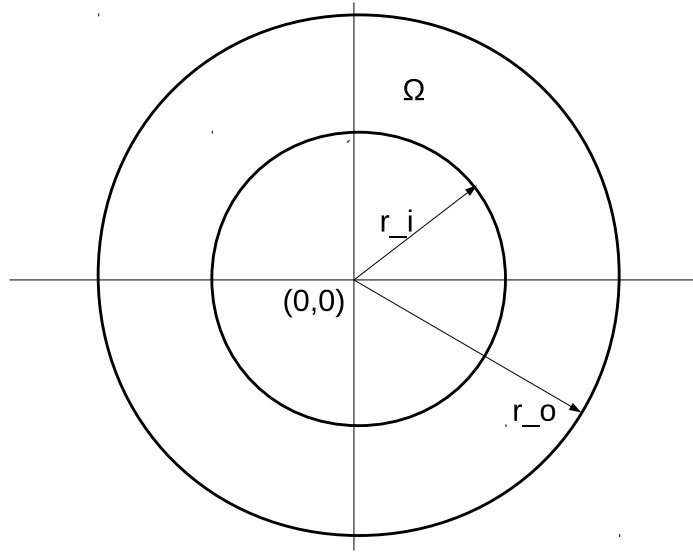


Figure 2: Annular domain with concentric circles

The first problem for validation is a simple annular domain with two circles as the boundaries as shown in fig. 2. The potential u is known beforehand and equal to $x + y$ and $g = u$. Two choices for the velocity field ν are considered:

$$\begin{aligned} \nu_1([x, y]) &:= [x, y], \\ \nu_2([x, y]) &:= [x/\sqrt{x^2 + y^2}, y/\sqrt{x^2 + y^2}]. \end{aligned} \quad (5.1)$$

For both these choices of velocity fields, we can analytically compute the boundary formula as follows:

$$u = x + y \implies \nabla u = [1, 1] \implies \|\nabla u\|^2 = 2. \quad (5.2)$$

Since we are dealing with circles, we can rewrite the velocity fields in polar coordinates:

$$\begin{aligned} \nu_1([r \cos(\theta), r \sin(\theta)]) &= [r \cos(\theta), r \sin(\theta)], \\ \nu_2([r \cos(\theta), r \sin(\theta)]) &= [\cos(\theta), \sin(\theta)]. \end{aligned} \quad (5.3)$$

¹Complete code can be found at <https://gitlab.ethz.ch/ppanchal/fsc.git>

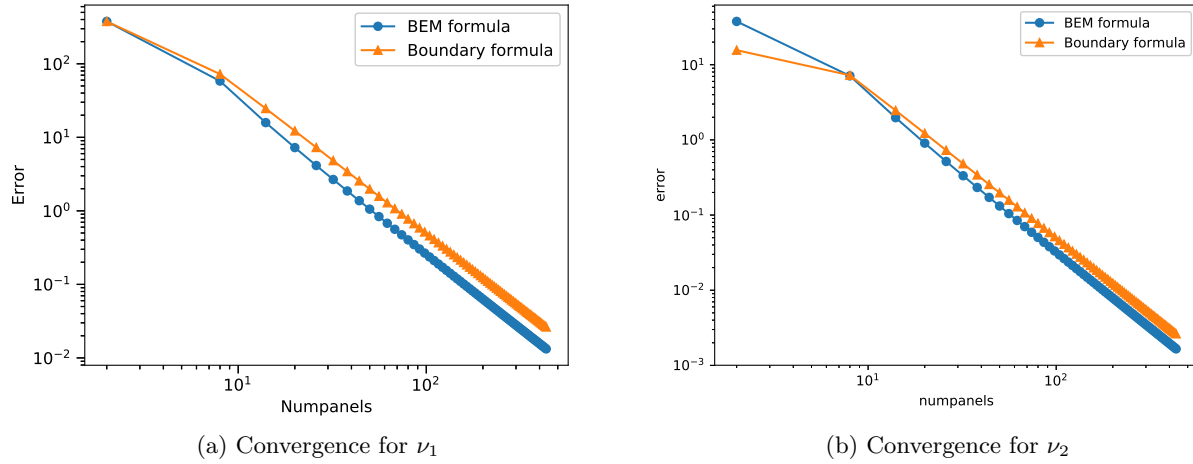


Figure 3: Absolute error plots for model problem 1

The normal vector for the outer circle is $[\cos(\theta), \sin(\theta)]$ and for the inner circle is $[-\cos(\theta), -\sin(\theta)]$. For $u = g$, the boundary formula becomes:

$$\begin{aligned}
 &= \frac{1}{2} \int_{\Gamma_0} \|\nabla u\|^2 \nu(\hat{x}) \cdot \hat{\mathbf{n}}(\hat{x}) d\Gamma_0(\hat{x}) \\
 &= r_o \int_{\theta=0}^{2\pi} r_o d\theta - r_i \int_{\theta=0}^{2\pi} r_i d\theta = 2\pi(r_o^2 - r_i^2); \quad \nu = \nu_1 \\
 &= r_o \int_{\theta=0}^{2\pi} d\theta - r_i \int_{\theta=0}^{2\pi} d\theta = 2\pi(r_o - r_i); \quad \nu = \nu_2.
 \end{aligned} \tag{5.4}$$

The absolute errors are plotted in figures 3a and 3b for both the boundary and BEM formula. As seen for both velocity fields, both BEM and boundary formulas show algebraic convergence with asymptotic slopes given in the table below:

Velocity	ν_1	ν_2
BEM	-2.039	-2.039
Boundary	-1.997	-1.997

5.1.2 Model Problem 2

We consider an annular domain with two circles as shown in figure 4

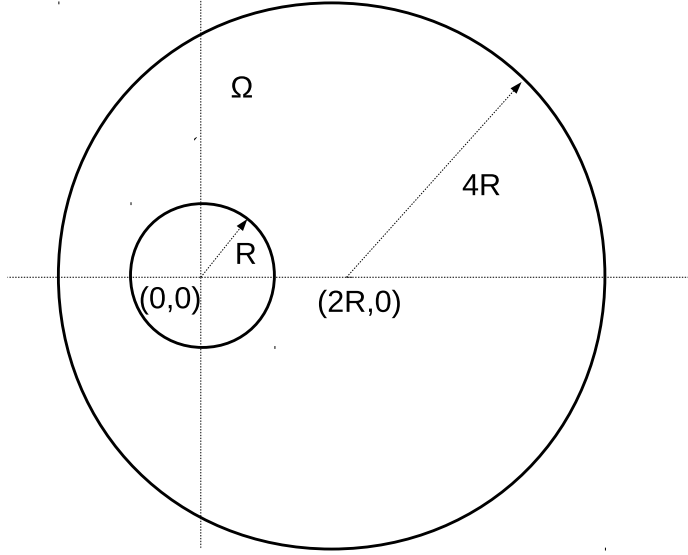


Figure 4: Annular domain with non concentric circles

The potential is known beforehand and is equal to $u([x, y]) = \log(\sqrt{x^2 + y^2})$. Two choices for the velocity field ν are considered at the inner circle:

$$\begin{aligned} \nu_1([x, y]) &:= [x, 0], \\ \nu_2([x, y]) &:= [1, 0]. \end{aligned} \quad (5.5)$$

At the outer circle, the velocity field is zero for both the choices and the choice of u makes the inner circle an equipotential surface. We can use $g = u = \log(\sqrt{x^2 + y^2})$ or we can use the following function g :

$$g = \begin{cases} \log(R) & \text{Inner circle} \\ \log(\sqrt{x^2 + y^2}) & \text{Outer circle} \end{cases}$$

It is easy to calculate the integrals in the boundary formula for both choices of g . We show it for the latter case ($u \neq g$). Since the velocity field is zero on the outer circle and g is constant on the inner circle ($\nabla g = 0$), we can simplify the boundary formula:

$$\begin{aligned} &= \frac{1}{2} \int_{\partial\Omega} ((\nabla g - \nabla u(\Omega)) \cdot n) (\nabla u(\Omega) \cdot n) \nu \cdot n \, dS + \frac{1}{2} \int_{\partial\Omega} \nabla g \cdot \nabla u(\Omega) \nu \cdot n \, dx \\ &= \frac{1}{2} \int_{\text{inner circle}} ((\nabla g - \nabla u(\Omega)) \cdot n) (\nabla u(\Omega) \cdot n) \nu \cdot n \, dS + \frac{1}{2} \int_{\text{inner circle}} \nabla g \cdot \nabla u(\Omega) \nu \cdot n \, dx \\ &= -\frac{1}{2} \int_{\text{inner circle}} (\nabla u(\hat{x}) \cdot \hat{\mathbf{n}}(\hat{x}))^2 \nu(\hat{x}) \cdot \hat{\mathbf{n}}(\hat{x}) \, d\Gamma_0(\hat{x}). \end{aligned} \quad (5.6)$$

For both these choices of velocity fields, we can analytically compute the formula above. Due to the presence of $x^2 + y^2$ in the potential, we switch to polar coordinates:

$$\begin{aligned} \nabla u &= \frac{\partial u}{\partial r} \hat{r} + \frac{\partial u}{r \partial \theta} \hat{\theta}, \quad u([r \cos(\theta), r \sin(\theta)]) = \log(r) \\ \implies \nabla u \cdot \hat{\mathbf{n}} &= -\frac{1}{r}, \quad \hat{\mathbf{n}} = -\hat{r} \quad \text{On the inner circle.} \end{aligned} \quad (5.7)$$

The boundary formula gives:

$$\begin{aligned}
&= -\frac{1}{2} \int_{\text{inner circle}} \|\nabla u(\hat{x}) \cdot \hat{\mathbf{n}}(\hat{x})\|^2 \nu(\hat{x}) \cdot \hat{\mathbf{n}}(\hat{x}) \, d\Gamma_0(\hat{x}) \\
&= \frac{1}{2} \int_{\theta=0}^{2\pi} \frac{1}{r_i^2} \nu([r_i \cos(\theta), r_i \sin(\theta)]) \cdot (\cos(\theta)\hat{i} + \sin(\theta)\hat{j}) \, r_i \, d\theta \\
&= \frac{1}{2r_i} \int_{\theta=0}^{2\pi} \nu([r_i \cos(\theta), r_i \sin(\theta)]) \cdot (\cos(\theta)\hat{i} + \sin(\theta)\hat{j}) \, d\theta \\
&= \frac{1}{2} \int_{\theta=0}^{2\pi} \cos(\theta)^2 \, d\theta = \frac{\pi}{2}, \quad \nu = \nu_1, \\
&= \frac{1}{2r_i} \int_{\theta=0}^{2\pi} \cos(\theta) \, d\theta = 0, \quad \nu = \nu_2.
\end{aligned} \tag{5.8}$$

Using the values calculated above, we plot the absolute errors for the BEM and boundary formulas. We see the same asymptotic convergence rates as seen in fig. 5a and 5b.

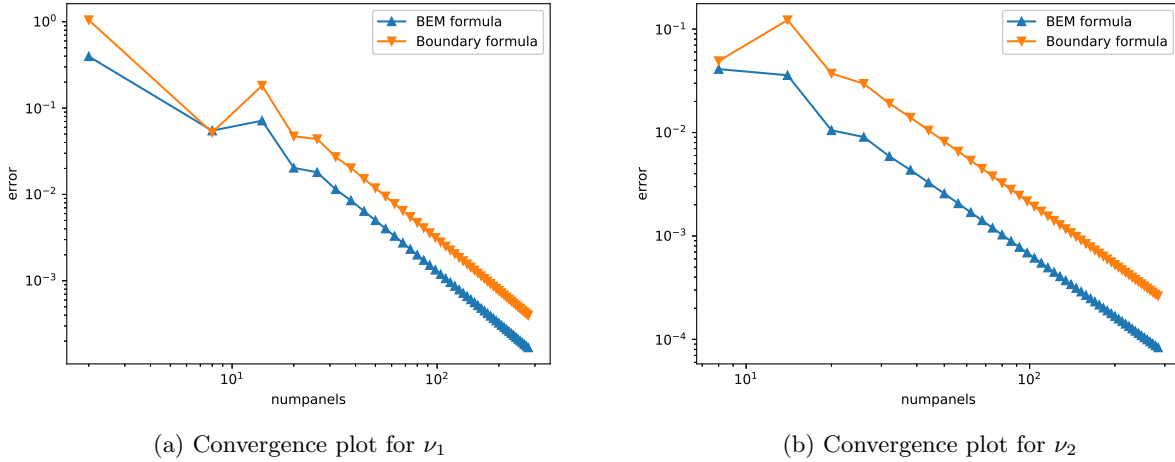
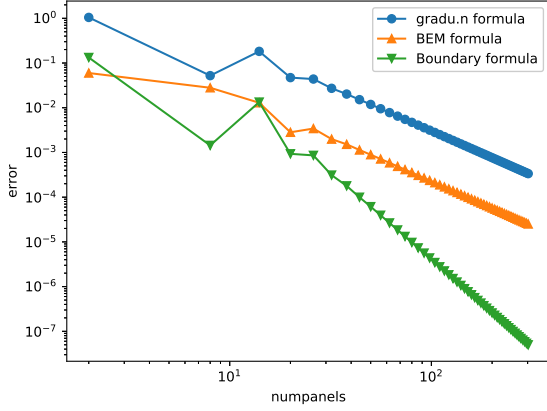


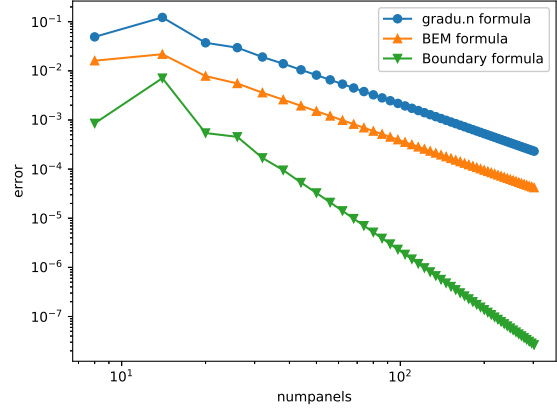
Figure 5: Absolute error plots for model problem 2 with $u \neq g$, $\nabla g = 0$ on inner circle

The above computations can be done using $u = g$ where for ν_1 and ν_2 we get $-\frac{\pi}{2}$ and 0 respectively. Figures 6a and 6b show the absolute error plots for both the velocity fields. In this case the boundary formula shows a better convergence rate than the BEM formula which gives the same asymptotic rate of convergence as the $\nabla u \cdot n$ formula. This indicates some simplification that happens when $u = g$.

Note: We can compare with the $\nabla u \cdot n$ formula in this example because as seen in the previous case with $u \neq g$, we get the same absolute values for the shape gradient.



(a) Convergence plot for ν_1



(b) Convergence plot for ν_2

Figure 6: Absolute error plots for model problem 2 with $u = g$

The asymptotic slopes for the plots are summarized in the following table:

Velocity, B.C.	$\nu_1, u \neq g$	$\nu_2, u \neq g$	$\nu_1, u = g$	$\nu_2, u = g$
BEM	-1.970	-1.973	-1.949	-1.976
Boundary	-1.974	-1.982	-3.918	-3.884
$\nabla u \cdot n$	N.A.	N.A.	-1.966	-1.954

5.1.3 Model Problem 3

Comparing the BEM and Boundary formula from eq. (2.60) and (4.29) respectively, we see that the derivatives of the velocity field ν appear only in the BEM formula. If the formulas are equivalent, a change in only the derivatives of the velocity field at the boundary should not change the shape gradient value. This model problem is designed to specifically test that. We have the same annular domain shown in fig. 2. The potential u is given as $u = x + y$ and we have $g = u$. We modify the velocity fields used in model problem 1 as follows:

$$\nu_1([x, y]) = \begin{cases} [x + x^2 + y^2 - r_i^2, y + x^2 + y^2 - r_i^2] & \text{Inner circle} \\ [x + x^2 + y^2 - r_o^2, y + x^2 + y^2 - r_o^2] & \text{Outer circle} \end{cases} \quad (5.9)$$

$$\nu_2([x, y]) = \begin{cases} [x/\sqrt{x^2 + y^2} + x^2 + y^2 - r_i^2, y/\sqrt{x^2 + y^2} + x^2 + y^2 - r_i^2] & \text{Inner circle} \\ [x/\sqrt{x^2 + y^2} + x^2 + y^2 - r_o^2, y/\sqrt{x^2 + y^2} + x^2 + y^2 - r_o^2] & \text{Outer circle} \end{cases} \quad (5.10)$$

Notice that the velocity fields give the same pointwise values at the boundary but have different gradients at the boundary. Using these velocity fields does not change the value obtained using the Boundary formula, calculated in model problem 1, using which we get the absolute error plots. We see in fig. 7a and 7b that for both modified velocity fields, the BEM formula converges to the right value. This is numerical evidence for the equivalence of the formulas, implying that the BEM formula can be converted to Hadamard form $\int_{\Gamma} \dots (\nu \cdot n) dS$. The asymptotic slopes are summarized in the following table:

Velocity	ν_1	ν_2
BEM	-2.037	-2.042
Boundary	-1.998	-1.997

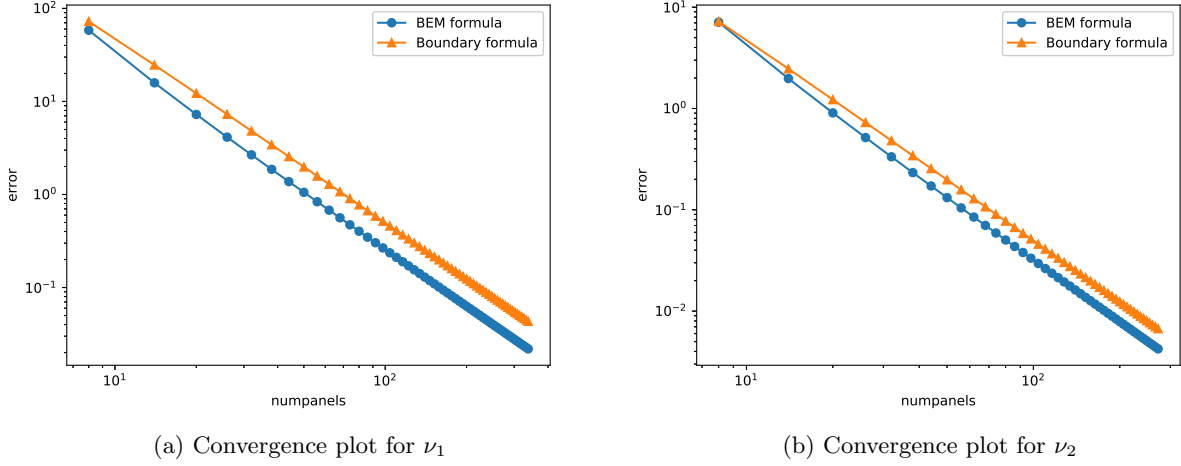


Figure 7: Convergence plots for model problem 3

5.2 Comparison of BEM and boundary formula

For testing the convergence rates, we look at the dual norm. Since the space $C^1(\mathbb{R}^d; \mathbb{R}^d)$ is infinite dimensional and reflexive, we use two simplifications [8, Ch. 2, Sec. 2.3]:

First, we consider an operator norm over a finite dimensional space of vector fields of the form:

$$\nu([x, y]) = \sum_{1 \leq m_1, m_2, n_1, n_2 \leq M} \lambda_{m_1, n_1} \begin{bmatrix} v(x, y, m_1, n_1) \\ 0 \end{bmatrix} + \lambda_{m_2, n_2} \begin{bmatrix} 0 \\ v(x, y, m_2, n_2) \end{bmatrix}. \quad (5.11)$$

Second, we use $H^1(D)$ norm instead of $C^1(\mathbb{R}^d; \mathbb{R}^d)$ norm as it is more tractable computationally. The basis for this finite dimensional space of vector fields is given as:

$$V = \{v(x, y, m, n) \mathbf{e}_j : 1 \leq m, n \leq M, j \in \{1, 2\}\}, M \in \mathbb{N}. \quad (5.12)$$

We use two choices for the function $v(x, y, m, n)$:

$$v(x, y, m, n) = \sin(mx) \sin(ny) \text{ or } \cos(mx) \cos(ny) \quad (\text{Sine/Cosine}), \quad (5.13)$$

$$v(x, y, m, n) = x^{m-1} y^{n-1} \quad (\text{Polynomial}). \quad (5.14)$$

For sinusoidal $v(x, y, m, n)$ we can see that for $M \rightarrow \infty$ the basis defined in eq. (5.12) becomes a basis of the space $C_0^1(D; \mathbb{R}^2)$ and for a polynomial $v(x, y, m, n)$, it becomes a basis of $C^1(\mathbb{R}^2; \mathbb{R}^2)$. The domain D is a sufficiently large square such that its edges are integer multiples of 2π . D has to be large enough to contain all domains Ω . The error is defined using dual norm:

$$err^{BEM} = \max_{\|\nu\|_{H^1(D)}=1} \left(\frac{d\mathcal{J}}{d\Omega}(\Omega; \nu) - \frac{d\mathcal{J}}{d\Omega}(\Omega, h; \nu)^{BEM} \right), \quad (5.15)$$

$$err^{Bdry} = \max_{\|\nu\|_{H^1(D)}=1} \left(\frac{d\mathcal{J}}{d\Omega}(\Omega; \nu) - \frac{d\mathcal{J}}{d\Omega}(\Omega, h; \nu)^{Bdry} \right). \quad (5.16)$$

In the expression for error, the term on left is the exact shape gradient value and the one on the right is the value computed at some refinement level h using the BEM formula or the Boundary formula (Bdry). On an abstract level, we have the following maximization problem:

$$val = \max_{\|\nu\|_{H^1(D)}=1} f(\nu),$$

which has an equivalent Lagrangian formulation given as:

$$val = \max_{\nu \in C^1(\mathbb{R}^2; \mathbb{R}^2)} \min_{\alpha \in \mathbb{R}} (f(\nu) + \alpha (\|\nu\|_{H^1(D)}^2 - 1)) .$$

α is the Lagrangian multiplier which appears along with the constraint term. We differentiate the Lagrangian to find the stationary points. We assume that the functional f is linear in ν :

$$f(\nu') + 2 \alpha \langle \nu, \nu' \rangle_{H^1(D)} = 0 \quad \forall \nu' \in C^1(\mathbb{R}^2; \mathbb{R}^2) .$$

Since we are only working with a finite dimensional space of vector fields V , we can write the above in algebraic form:

$$\begin{aligned} f(\nu') + 2 \alpha \langle \nu, \nu' \rangle_{H^1(D)} &= 0 \quad \forall \nu' \in V, \nu \in V \\ \implies \vec{f} + 2 \alpha G \vec{z} &= 0 . \end{aligned}$$

In the algebraic form, \vec{f} is the vector of the functional values for all basis elements from the space V , i.e. $\vec{f} = \{f(\nu_i)\}$ where $\{\nu_i\}$ is the basis. G is the Gramian matrix for the finite dimensional set V with respect to the $H^1(D)$ norm, given as $G_{i,j} = \langle \nu_i, \nu_j \rangle_{H^1(D)}$. \vec{z} represents the coefficients of the solution ν of the optimization problem with respect to the basis of V . Using the vector equation above we get \vec{z} as:

$$\vec{z} = -\frac{1}{2\alpha} G^{-1} \vec{f}$$

Since $\|\nu\|^2 = 1$ we get:

$$\begin{aligned} \vec{z}^T G \vec{z} &= \frac{1}{4\alpha^2} \vec{f}^T G^{-1} \vec{f} = 1 \\ \implies \alpha &= \frac{1}{2} \sqrt{\vec{f}^T G^{-1} \vec{f}} \\ \implies val &= \vec{f}^T \vec{z} = \sqrt{\vec{f}^T G^{-1} \vec{f}} \end{aligned} \tag{5.17}$$

We define the column vectors \vec{f} in our case as:

$$\left\{ \frac{d\mathcal{J}}{d\Omega}(\Omega; \nu_i) - \frac{d\mathcal{J}}{d\Omega}(\Omega, h; \nu_i)^{BEM} \right\}_{i=1}^{dim(V)}$$

Knowing the Gramian Matrix G for the finite dimensional basis of velocity fields, with respect to the $H^1(D)$ norm, we can compute the error at any refinement level using eq. (5.17). Here we do experiments on both smooth (model problem 4 and 5) and non-smooth domains (model problem 6 onwards).

5.2.1 Model Problem 4

We have an annular domain made up of two squares as shown in the figure 8. The boundary conditions are given as $g = 0$ on inner square and $g = 1$ on the outer square with $\nabla g = 0$ on both boundaries. We plot the dual norm error for both sinusoidal and polynomial velocity fields. Fig. 9 shows the results for a quadrature order of 16 and fig. 10 shows them with order 32. Since analytical solution for this domain is not available, the converged value is calculated using 8000 panels for order 16 and with 4000 panels for order 32. Since the domain has piecewise linear boundary, the parametric mesh is equivalent to a linear mesh in this case.

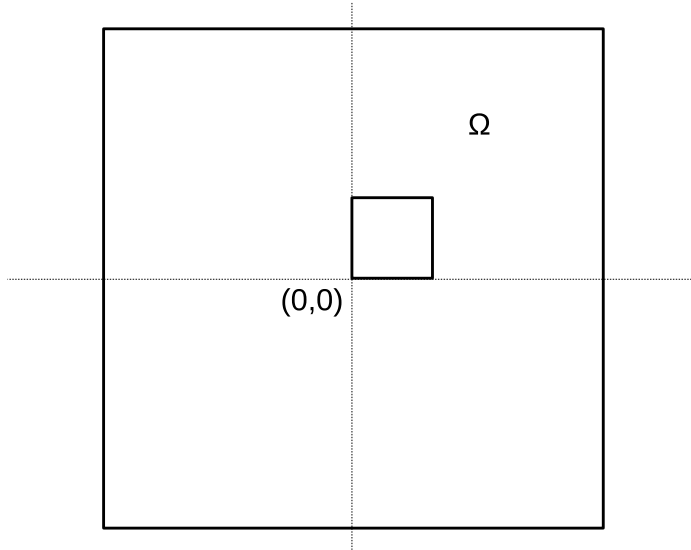


Figure 8: Annular domain with squares

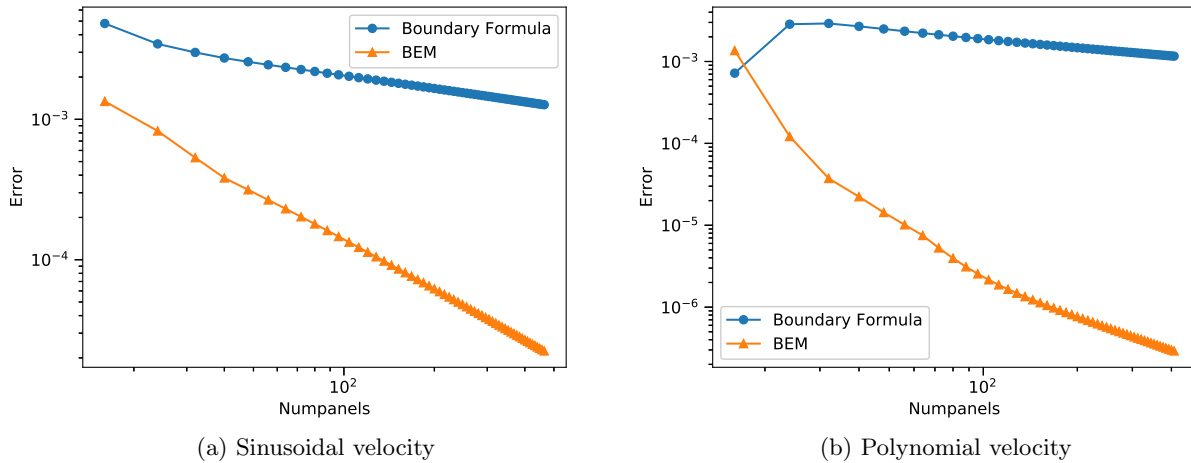


Figure 9: Dual norm error plots for annular square domain with quadrature order = 16

We see that for both choices of the velocity field and quadrature order, BEM formula shows a higher convergence rate than the Boundary formula. This can be attributed in part to the presence of sharp corners in the domain which introduce a singularity in the solution as discussed in the lecture document for NUMPDE using harmonic corner singular functions [4, Ch. 5, Thm 5.4.6]. This is discussed further in the next experiment. The asymptotic slopes (ignoring the initial transient behaviour) for all the plots are summarized in the following table:

Velocity and order	Poly. 16	Sin. 16	Poly. 32	Sin. 32
BEM	-1.373	-1.188	-1.406	-1.231
Boundary	-0.334	-0.335	-0.336	-0.347

It is also possible to find the total force on the body using shape gradient formulas when $\nabla g = 0$. In

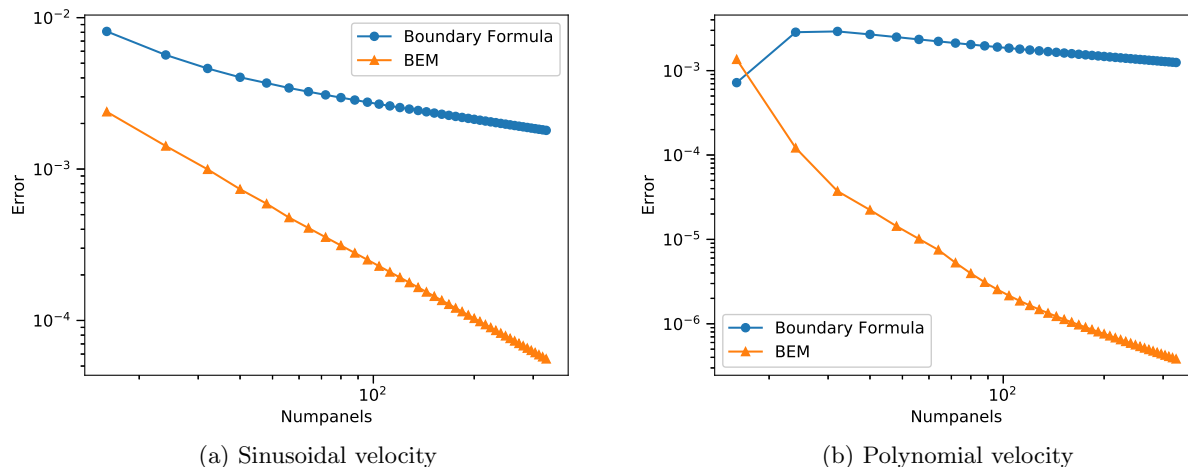


Figure 10: Dual norm error plots for annular square domain with quadrature order = 32

such cases, the boundary shape gradient formula becomes:

$$-\frac{1}{2} \int_{\partial\Omega} (\nabla u \cdot n)^2 \nu \cdot n \, dS. \quad (5.18)$$

By using constant velocity fields in the x and y directions, the shape gradient formula reduces to the x and y force components:

$$\begin{aligned} \nu = [1, 0] &\implies -\frac{1}{2} \int_{\partial\Omega} (\nabla u \cdot n)^2 n_x \, dS = F_x, \\ \nu = [0, 1] &\implies -\frac{1}{2} \int_{\partial\Omega} (\nabla u \cdot n)^2 n_y \, dS = F_y, \end{aligned} \quad (5.19)$$

where n_x and n_y are the x and y components of the unit normal field respectively. Information about the convergence rates for the F_x and F_y is also contained in the dual norm error plots for the polynomial velocity field as the polynomial velocity field basis contains the constant velocity fields used in eq. (5.19). Hence the convergence rate for the total force is much better with the BEM formula in this example.

5.2.2 Model Problem 5

We have a simply connected domain with a re-entrant corner as shown in the figure 11. We know the potential u beforehand:

$$u(r, \phi) = r^{\frac{2}{3}} \sin\left(\frac{2}{3}\phi\right)$$

The potential u is the harmonic corner singular function we talked about in the previous experiment, plotted in fig. 12. For g , we use the same function as u in one case and $g(r, \phi) = r \sin(\frac{2}{3}\phi)$ in the other. The second choice of g gives the same boundary conditions and hence the same solution for the Neumann Trace. But the two choices of g differ in one important aspect: smoothness. For $g = u$, we can verify that $\|\nabla g\| \rightarrow \infty$ at the origin as seen in fig. 13, whereas it is well behaved for the other case. This singularity is also present in the Neumann Trace but it can be verified that it is still in $L^2(\partial\Omega)$.

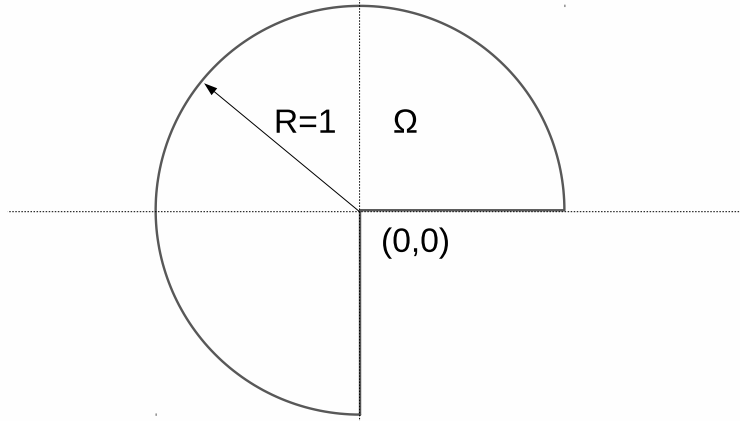


Figure 11: Domain with re-entrant corner at the origin

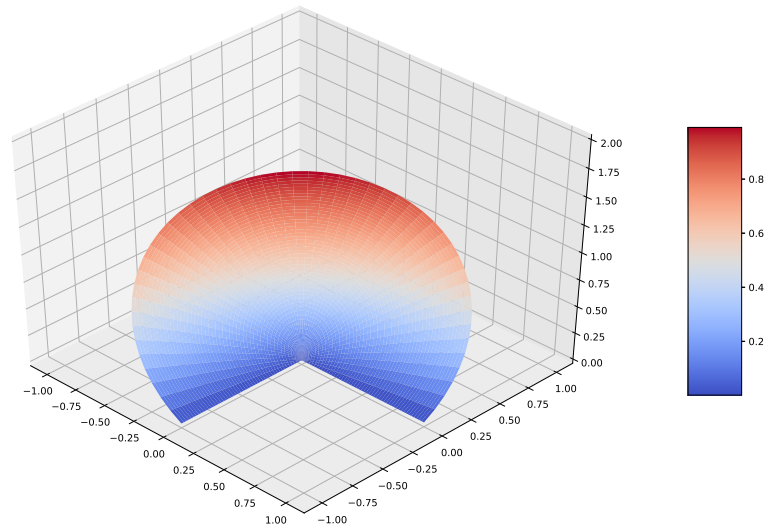


Figure 12: Surface plot for $u = r^{\frac{2}{3}} \sin(\frac{2}{3}\phi)$

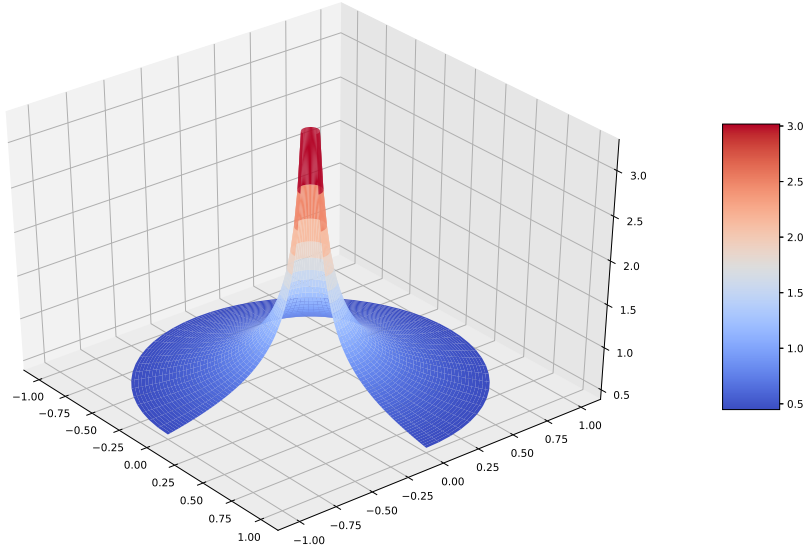
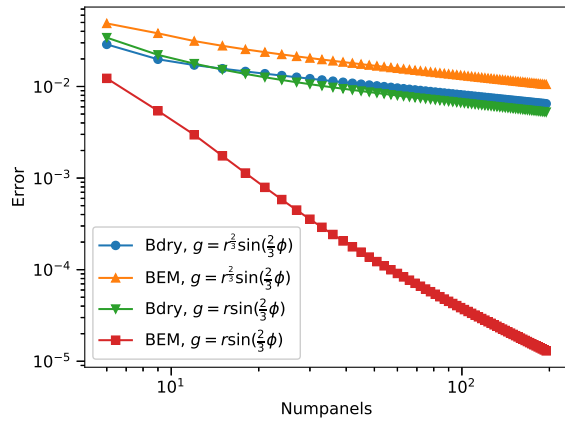


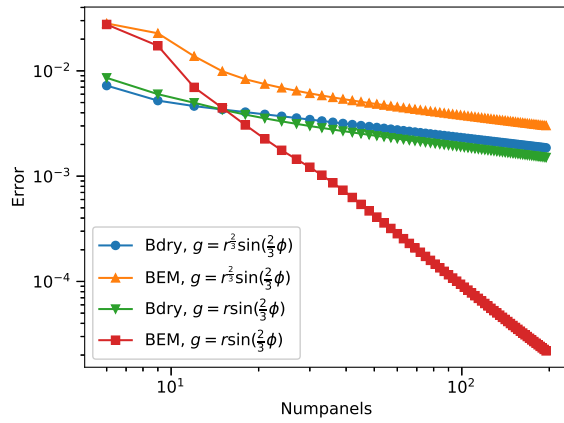
Figure 13: Surface plot for $\|\nabla u\|^2$ for $u = r^{\frac{2}{3}} \sin(\frac{2}{3}\phi)$

Like in the previous experiment, we have a singularity in the Neumann Trace solution. In this experiment we see that the smoothness of g is an important factor as well. The convergence rate for BEM formula is better than the Boundary formula only when we have a smooth g , which is confirmed by both polynomial and cosine velocity fields as seen in fig. 14. They have same asymptotic convergence rates when g is not smooth. The same results are obtained for a higher quadrature order, shown in fig. 15. In contrast, performance of the Boundary formula seems unaffected by the improvement in smoothness of g . This experiment reveals two conditions where BEM formula is better than the Boundary formula: a singularity in the Neumann Trace solution because of sharp corners in the domain and a smooth g . The experiment also provides evidence for the problems with the Boundary formula or the total force formula obtained from Maxwell Stress Tensor: It is doomed when we have a singularity in the Neumann Trace (even when it is in L^2). Note that in the previous experiment ∇g was zero and the BEM formula was much better, which agrees with the observations in this experiment.

Note: The converged values for the shape gradient are computed in Mathematica using the "Local-Adaptive" quadrature method as the solution has a singularity.

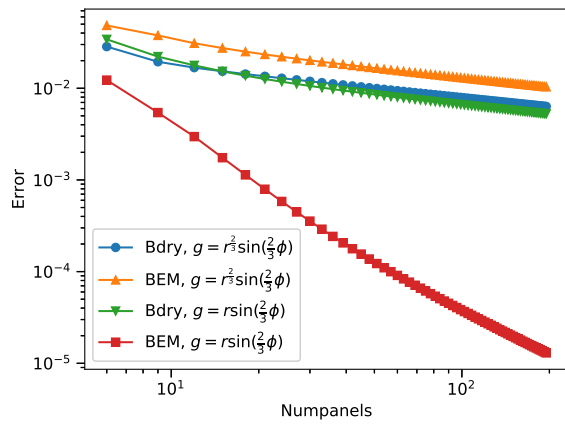


(a) Polynomial field

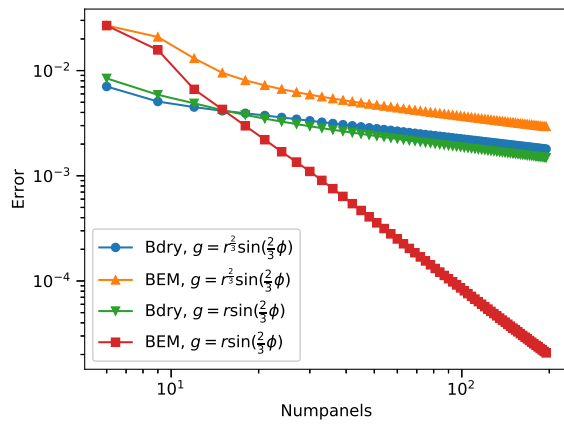


(b) Cosine field

Figure 14: Dual norm error plots for pacman domain with quadrature order = 16



(a) Polynomial field



(b) Cosine field

Figure 15: Dual norm error plots for pacman domain with quadrature order = 32

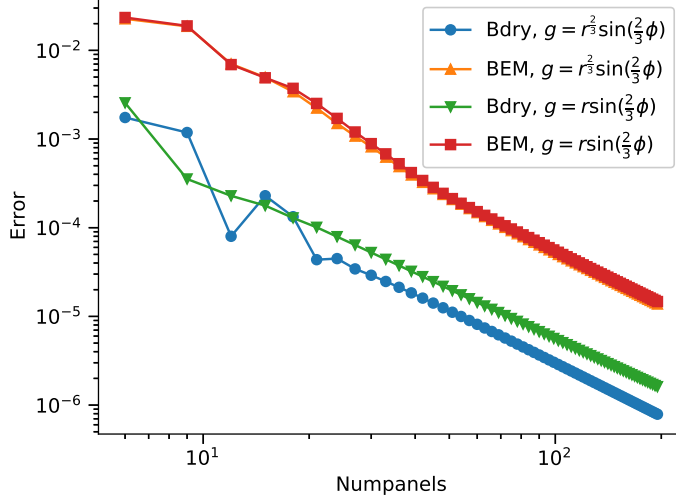


Figure 16: Dual norm error plots for pacman domain, sinusoidal velocity field and quadrature order = 16

The asymptotic slopes for fig. 14 and 15 (ignoring the initial transient behaviour) are summarized in the following tables:

Velocity, g	Poly., smooth	Poly., non-smooth	Cos., smooth	Cos., non-smooth
BEM, 16	-1.655	-0.343	-2.179	-0.347
Boundary, 16	-0.355	-0.335	-0.351	-0.332
BEM, 32	-1.655	-0.344	-2.120	-0.346
Boundary, 32	-0.355	-0.335	-0.350	-0.332

Using a sinusoidal velocity field instead of cosine reveals something interesting. As seen in fig. 16, the sinusoidal velocity field dramatically improves the convergence rate of the BEM formula for a non smooth g and also improves the convergence rate of the Boundary formula for both smooth and non smooth g . This is because a sinusoidal velocity field masks the singularity of the solution at the origin. This is evidence for the claim that the singularity of the solution is in part responsible for the trends observed earlier. The asymptotic slopes for fig. 16 (ignoring the initial transient behaviour) are summarized in the following table:

g	smooth	non-smooth
BEM	-1.947	-1.981
Boundary	-1.852	-1.980

We perform another experiment with $g = r^{\frac{3}{4}} \sin(\frac{2}{3}\phi)$ which does not change the boundary conditions or the Neumann trace. The idea is to make $g \neq u$ while still keeping $\|\nabla g\| \rightarrow \infty$ at the origin and the same Neumann Trace solution. As seen with a non smooth g earlier, the BEM formula doesn't offer a good convergence rate, which is what we observe here as seen in fig. 17. But here we see that BEM formula is the only one that converges with asymptotic slope equal to -0.427 and -0.451 for polynomial and cosine field respectively. This again indicates towards some simplifications in the Boundary formula when $u = g$ as it was able to converge with a similar asymptotic rate in that case but fails to do so in this case where $u \neq g$.

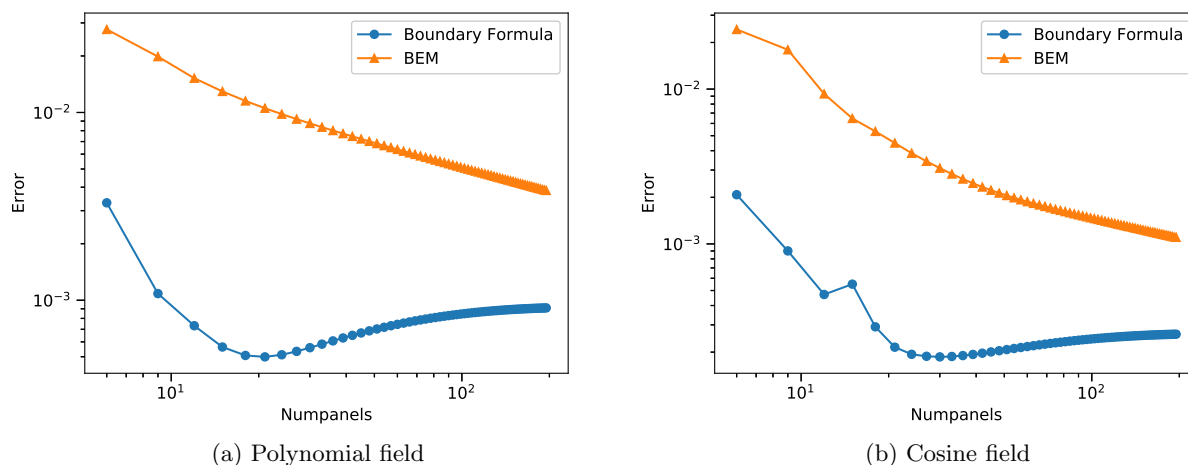


Figure 17: Convergence plots for pacman domain with $g = r^{\frac{3}{4}} \sin(\frac{2}{3}\phi)$ and quadrature order = 16

5.2.3 Model Problem 6

We have an annular domain with two concentric circles as shown in figure 2. We have the following Dirichlet boundary conditions:

$$g = \begin{cases} 0 & \text{Outer boundary} \\ \frac{1}{2}(1 + \cos(2\phi) + 2 \sin(\phi)) & \text{Inner boundary} \end{cases}$$

For the annular circle case we know the analytic solution whose general form is :

$$u(r, \phi) = a_0 + b_0 \log(r) + \sum_{i=1} (a_i r^i + b_i r^{-i}) \cos(i\phi) + (c_i r^i + d_i r^{-i}) \sin(i\phi) .$$

We can easily find the solution using the boundary conditions. It is very smooth as shown in fig. 18

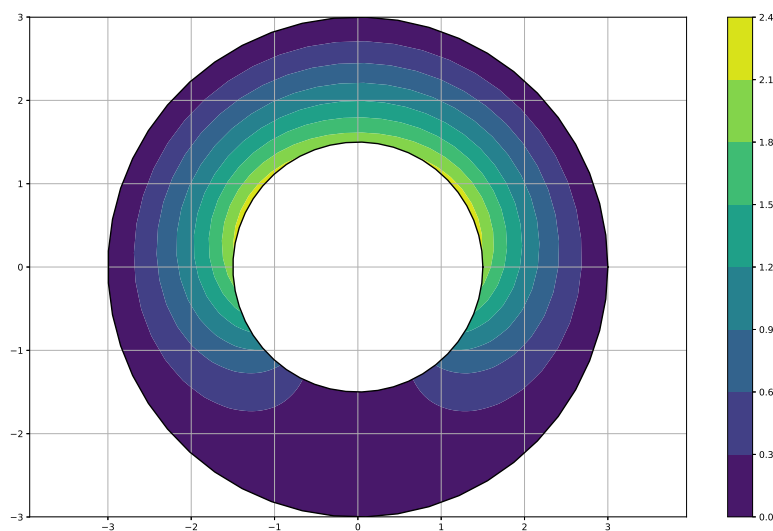


Figure 18: Solution for model problem 6

We plot the dual norm errors for both sinusoidal and polynomial velocity fields, using a quadrature order of 16 and 32. The results are shown in figures 19 and 20. The results indicate a similar asymptotic convergence rate. This indicates that the two formulas are equivalent assuming sufficient smoothness everywhere. Also notice $u \neq g$ in this experiment and BEM formula stays ahead by a small factor in all the cases.

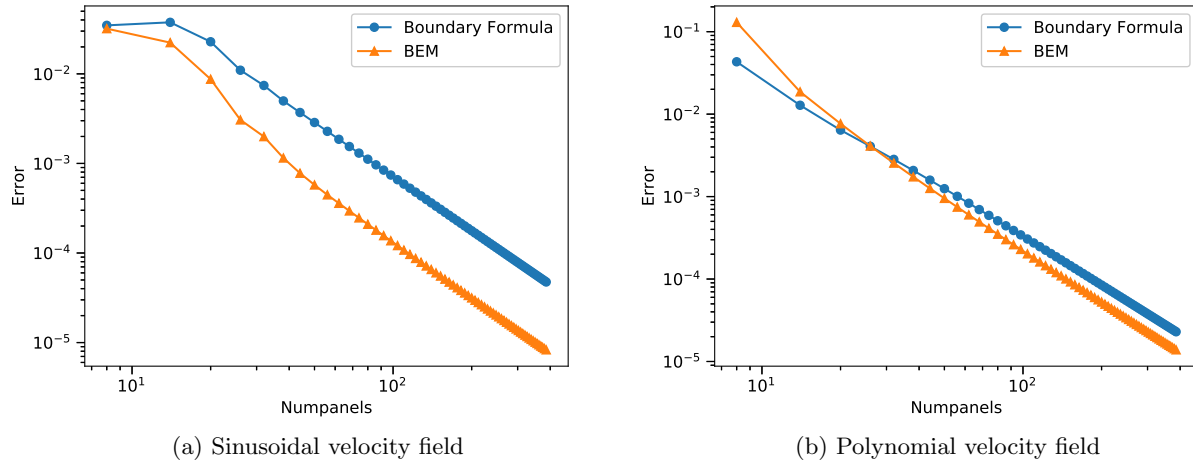


Figure 19: Convergence plots for different velocity fields with quadrature order = 16 and parametric mesh

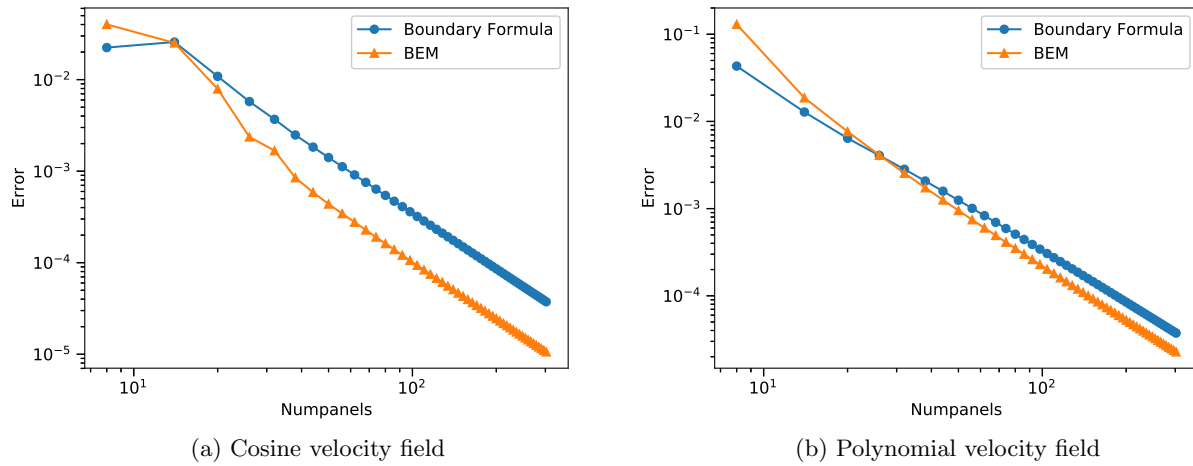


Figure 20: Convergence plots for different velocity fields with quadrature order = 32 and parametric mesh

The asymptotic slopes (ignoring the initial transient behaviour) are summarized in the following tables:

Velocity	Trigonometric	Polynomial
BEM, 16	-2.041 (Sin)	-2.042
Boundary, 16	-2.005 (Sin)	-1.976
BEM, 32	-2.042 (Cos)	-2.047
Boundary, 32	-2.012 (Cos)	-1.973

5.2.4 Model Problem 7

We consider the domain from fig. 4. We have $u = \log(r)$ and two choices for g . One of them is simply $g = u$ and in the other one, we add artificial gradients to g at the boundary as follows:

$$g = \begin{cases} \log(R) & \text{Inner circle} \\ \log(r) + (x - 2R)^2 + y^2 - 16R^2 & \text{Outer circle} \end{cases}$$

We are interested in seeing the effect of $g = u$ on the convergence of the shape gradient formulas when the Neumann Trace is smooth. We plot the dual norm errors for both cosine and polynomial velocity fields, using quadrature order = 16. The results are shown in fig. 21.

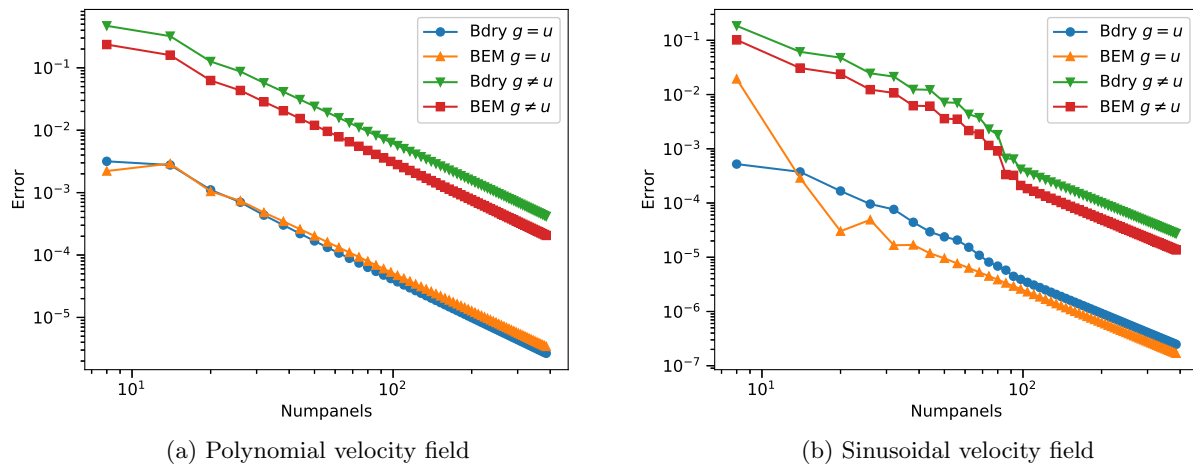


Figure 21: Convergence plots for different velocity fields

We see that $u = g$ does offer some advantage to the boundary formula in the smooth case as seen in another experiment earlier. But the advantage is just a small constant factor with the asymptotic convergence rates being similar as seen in the table below:

Velocity, B.C.	Poly., $u = g$	Poly., $u \neq g$	Sin., $u = g$	Sin., $u \neq g$
BEM	-1.998	-1.993	-1.992	-1.988
Boundary	-2.009	-1.993	-2.007	-1.987

5.2.5 Model Problem 8

We consider the annular domain from fig. 22 with two fourier kites given as:

$$\begin{aligned} \gamma_i(t) &= [0.5 - 0.8 \cos(\phi) - 0.3 \cos(2\phi), 0.5 + \sin(\phi)] \\ \gamma_o(t) &= [3.5 \cos(\phi) + 1.625 \cos(2\phi), 3.5 \sin(\phi)] \end{aligned}$$

We have $u = g = \log(r)$. We plot the dual norm errors for quadrature order 16, considering both polynomial and cosine velocity fields.

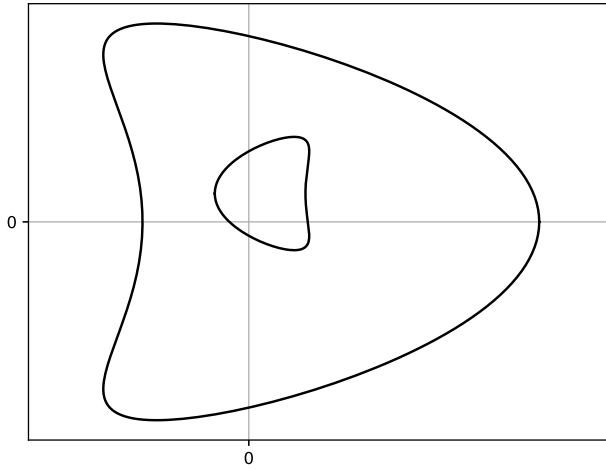


Figure 22: Annular domain with two Fourier kites

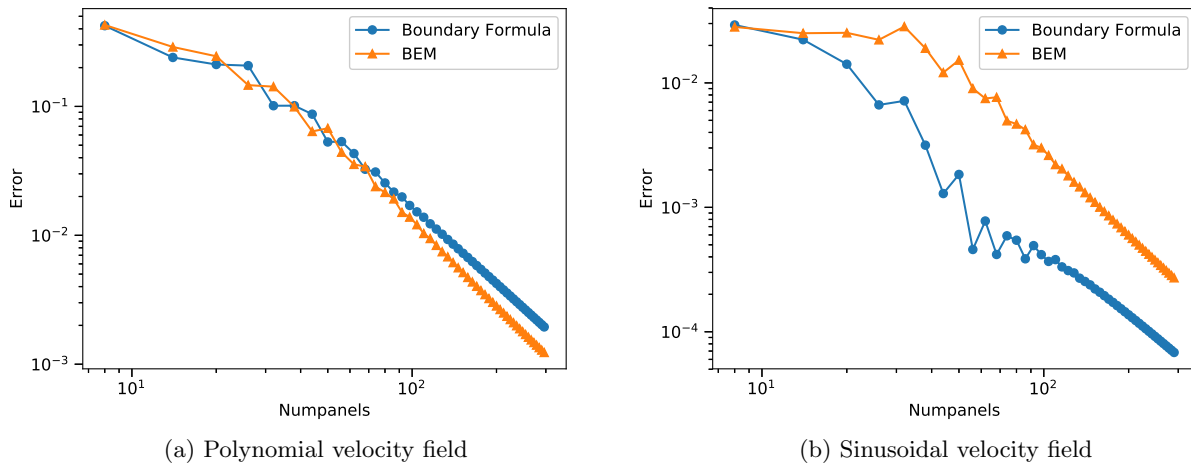


Figure 23: Convergence plots for different velocity fields

We see very similar asymptotic slopes summarized in the following table:

Velocity	Sin	Polynomial
BEM	-2.197	-2.172
Boundary	-1.711	-1.969

6 Conclusion and Outlook

The numerical experiments suggest that the BEM and boundary formulas have similar asymptotic convergence rates when the Neumann Trace of the Dirichlet BVP is smooth, although some slight differences of constant factors are present which may depend on whether g and u are equal or not. When the Neumann Trace is not smooth, as in domains with sharp corners, the regularity of the function g is the decisive factor: If g is smooth, the BEM formula has a much better convergence rate. This superiority of the BEM formula

disappears when regularity for g is lowered and its asymptotic rate of convergence matches the boundary formula. These trends can be explained by looking at the formulas. The BEM formula is continuous on the energy trace space $H^{-\frac{1}{2}}(\Gamma)$ in contrast to the boundary formula which is unbounded on $H^{-\frac{1}{2}}(\Gamma)$: If the Neumann Trace Ψ contains a singularity, the Boundary formula is destined to suffer whereas the BEM formula can still survive because of duality arguments, provided that g has sufficient regularity. With these results we can conclude that the new BEM formula would undoubtedly be better in case of conductors with sharp corners. The singularity in the solution because of sharp corners and $\nabla g = 0$ provide the perfect conditions for the BEM formula to shine. It could also prove to be better in other physical cases where the function g is usually smooth.

What remains to be done is finding a link between the shape gradient formula and the Maxwell stress tensor force formula for a general case ($\nabla g \neq 0$). In the case of conductors ($\nabla g = 0$) the shape gradient reduces to a very similar form but the link between them for a general case is obscure. The proof of equivalency of the two formulas is still an open problem but the numerical experiments suggest that they are equivalent, thus it should be possible. Other interesting directions include formulating the Dirichlet BVP in different ways and finding the shape gradient formulas using those constraints, for example a floating potential problem or Maxwell eddy current problem.

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A Incomplete proof of equivalency of BEM and Boundary formulas

Here I present some ideas which might be helpful while trying to prove the equivalency of the BEM and Boundary formulas on a smooth level. I should warn the reader that there may be some mistakes in the procedure. The general shape gradient formula from eq. (2.60), c here is just $\frac{1}{2}$:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \{ \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y}) \} p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) \kappa(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) + g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (A(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\
& \quad + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) (\nabla g(\hat{y}) \cdot \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x})
\end{aligned} \tag{A.1}$$

Using the expression for matrix A from eq. (2.36) and the expression for $\kappa(\hat{x}, \hat{y})$, given as:

$$\kappa(\hat{x}, \hat{y}) = \nabla_x \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{x}) + \nabla_y \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{y}) \tag{A.2}$$

We get the shape gradient as:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \{ \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y}) \} p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) (\nabla_x \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{x}) + \nabla_y \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) \\
& \quad + g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot ((\nabla \cdot \nu(\hat{y}) I - \nabla \nu(\hat{y})) \hat{\mathbf{n}}(\hat{y})) \\
& \quad + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) (\nabla g(\hat{y}) \cdot \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x})
\end{aligned} \tag{A.3}$$

Simplifying, we get:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x})(\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \{ \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \nu(\hat{y}) \} p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) (\nabla_x \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{x}) + \nabla_y \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) \\
& \quad - g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\
& \quad + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x})
\end{aligned} \tag{A.4}$$

The terms highlighted in red above can be written as:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x}) (\nabla \cdot (g(\hat{x})\nu(\hat{x})) - g(\hat{x})\nabla \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) (\nabla_y \cdot (G(\hat{x}, \hat{y})\nu(\hat{y})) - G(\hat{x}, \hat{y})\nabla \cdot \nu(\hat{y})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& = c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot (g(\hat{x})\nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_y \cdot (G(\hat{x}, \hat{y})\nu(\hat{y})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) - a_V(p, \Psi_0 \nabla \cdot \nu) - J(\Psi_0 \nabla \cdot \nu) \\
& = c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot (g(\hat{x})\nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_y \cdot (G(\hat{x}, \hat{y})\nu(\hat{y})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})
\end{aligned} \tag{A.5}$$

We have the following identity :

$$(\nabla_x \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{x})) \cdot \hat{\mathbf{n}}(\hat{y}) = \hat{\mathbf{n}}(\hat{y})^T \nabla_x \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{x}) = (\nabla_x \nabla_y G(\hat{x}, \hat{y}) \hat{\mathbf{n}}(\hat{y})) \cdot \nu(\hat{x}) \tag{A.6}$$

$$\nabla_x (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) = \nabla_x \nabla_y G(\hat{x}, \hat{y}) \hat{\mathbf{n}}(\hat{y}) + \nabla_x \hat{\mathbf{n}}(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) = \nabla_x \nabla_y G(\hat{x}, \hat{y}) \hat{\mathbf{n}}(\hat{y}) \tag{A.7}$$

$$\implies \nabla_x \cdot (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) \nu(\hat{x})) = \nabla_x (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) \nabla \cdot \nu(\hat{x}) \tag{A.8}$$

$$= (\nabla_x \nabla_y G(\hat{x}, \hat{y}) \hat{\mathbf{n}}(\hat{y})) \cdot \nu(\hat{x}) + \nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) \nabla \cdot \nu(\hat{x}) \tag{A.9}$$

The terms highlighted in yellow :

$$\begin{aligned}
& \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_x G(\hat{x}, \hat{y}) \cdot \nu(\hat{x}) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) (\nabla_x \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{x})) \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& \quad - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) (\nabla g(\hat{x}) \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& = \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) (\nabla_x \cdot (G(\hat{x}, \hat{y})\nu(\hat{x})) - G(\hat{x}, \hat{y})\nabla \cdot \nu(\hat{x})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) (\nabla_x \cdot (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})\nu(\hat{x})) - \nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})\nabla \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& \quad - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) (\nabla \cdot (g(\hat{x})\nu(\hat{x})) - g(\hat{x})\nabla \cdot \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& = \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_x \cdot (G(\hat{x}, \hat{y})\nu(\hat{x})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& \quad - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \nabla_x \cdot (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})\nu(\hat{x})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) \nabla \cdot (g(\hat{x})\nu(\hat{x})) d\Gamma_0(\hat{x}) - a_V(\Psi_0, p \nabla \cdot \nu) + a_K(p \nabla \cdot \nu) + \frac{1}{2} l(p \nabla \cdot \nu) \\
& = \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_x \cdot (G(\hat{x}, \hat{y})\nu(\hat{x})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& \quad - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \nabla_x \cdot (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})\nu(\hat{x})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& \quad - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) \nabla \cdot (g(\hat{x})\nu(\hat{x})) d\Gamma_0(\hat{x})
\end{aligned} \tag{A.10}$$

Using the simplifications above, the shape gradient formula becomes:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot (g(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_y \cdot (G(\hat{x}, \hat{y}) \nu(\hat{y})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_x \cdot (G(\hat{x}, \hat{y}) \nu(\hat{x})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \nabla_x \cdot (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) \nu(\hat{x})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) \nabla \cdot (g(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) (\nabla_y \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) \\
& - g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\
& + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})
\end{aligned} \tag{A.11}$$

The terms underlined in red above can be rearranged as follows:

$$\begin{aligned}
& \int_{\Gamma_0} \nabla_x \cdot \left(\int_{\Gamma_0} G(\hat{x}, \hat{y}) \Psi_0(\hat{y}) d\Gamma_0(\hat{y}) \nu(\hat{x}) \right) p(\hat{x}) d\Gamma_0(\hat{x}) \\
& - \int_{\Gamma_0} p(\hat{x}) \nabla_x \cdot \left(\int_{\Gamma_0} \nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) g(\hat{y}) d\Gamma_0(\hat{y}) \nu(\hat{x}) \right) d\Gamma_0(\hat{x}) \\
& = \int_{\Gamma_0} \nabla_x \cdot (\Psi_{SL}(\Psi_0)(\hat{x}) \nu(\hat{x})) p(\hat{x}) d\Gamma_0(\hat{x}) \\
& - \int_{\Gamma_0} p(\hat{x}) \nabla_x \cdot (\Psi_{DL}(g)(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& = \int_{\Gamma_0} \nabla \cdot \left((\Psi_{SL}(\Psi_0)(\hat{x}) - \Psi_{DL}(g)(\hat{x})) \nu(\hat{x}) \right) p(\hat{x}) d\Gamma_0(\hat{x})
\end{aligned} \tag{A.12}$$

Thus the shape gradient formula reduces to:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot (g(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_y \cdot (G(\hat{x}, \hat{y}) \nu(\hat{y})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& + \int_{\Gamma_0} \nabla \cdot \left((\Psi_{SL}(\Psi_0)(\hat{x}) - \Psi_{DL}(g)(\hat{x})) \nu(\hat{x}) \right) p(\hat{x}) d\Gamma_0(\hat{x}) \\
& - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) \nabla \cdot (g(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) (\nabla_y \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) \\
& - g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\
& + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})
\end{aligned} \tag{A.13}$$

We look closely at the adjoint equation:

$$\begin{aligned}
& a_V(p, v) + J(v) = 0 \quad \forall v \in H^{-\frac{1}{2}}(\Omega) \\
& \rightarrow \int_{\Gamma_0} \int_{\Gamma_0} v(\hat{y}) G(\hat{x}, \hat{y}) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) = -c \int_{\Gamma_0} v(\hat{x}) g(\hat{x}) d\Gamma_0(\hat{x}) \\
& \rightarrow \int_{\Gamma_0} \int_{\Gamma_0} v(\hat{y}) G(\hat{x}, \hat{y}) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) = \int_{\Gamma_0} v(\hat{x}) g'(\hat{x}) d\Gamma_0(\hat{x}), \quad g' = -c g
\end{aligned} \tag{A.14}$$

We look at the indirect first kind BEM formulation for the following Dirichlet problem:

$$\begin{aligned}
& \Delta u' = 0 \quad \text{in } \Omega, \quad u' = g' \quad \text{on } \partial\Omega \\
& \text{Trying } u' = \Psi_{SL}(f) \implies V(f) = g' \\
\implies & \int_{\Gamma_0} \int_{\Gamma_0} v(\hat{y}) G(\hat{x}, \hat{y}) f(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) = \int_{\Gamma_0} v(\hat{x}) g'(\hat{x}) d\Gamma_0(\hat{x}) \quad \forall v \in H^{-\frac{1}{2}}(\Omega)
\end{aligned} \tag{A.15}$$

The adjoint equation is exactly same as the indirect first kind variational formulation with $p = f$. We also know that $u'(x) = -c u(x)$:

$$\begin{aligned}
-c u(\hat{x}) &= \int_{\Gamma_0} G(\hat{x}, \hat{y}) p(\hat{y}) d\Gamma_0(\hat{y}), \quad x \in \Omega \\
\implies u(\hat{x}) &= -\frac{1}{c} \int_{\Gamma_0} G(\hat{x}, \hat{y}) p(\hat{y}) d\Gamma_0(\hat{y})
\end{aligned} \tag{A.16}$$

Using these identities, we get:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot (g(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_y \cdot (G(\hat{x}, \hat{y}) \nu(\hat{y})) p(\hat{x}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& + \int_{\Gamma_0} \nabla \cdot \left((\Psi_{SL}(\Psi_0)(\hat{x}) - \Psi_{DL}(g)(\hat{x})) \nu(\hat{x}) \right) p(\hat{x}) d\Gamma_0(\hat{x}) \\
& \quad - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) \nabla \cdot (g(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& \quad - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) (\nabla_y \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) \\
& \quad \quad - g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\
& \quad \quad + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})
\end{aligned} \tag{A.17}$$

The terms in red can be written as:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot (g(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_y \cdot \left(\int_{\Gamma_0} G(\hat{x}, \hat{y}) p(\hat{x}) d\Gamma_0(\hat{x}) \nu(\hat{y}) \right) d\Gamma_0(\hat{y}) \\
& \quad = c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot (g(\hat{x}) \nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& \quad + \int_{\Gamma_0} \Psi_0(\hat{y}) \nabla_y \cdot (-c u(\hat{y}) \nu(\hat{y})) d\Gamma_0(\hat{y}) \\
& \quad = c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot ((g(\hat{x}) - u(\hat{x})) \nu(\hat{x})) d\Gamma_0(\hat{x})
\end{aligned} \tag{A.18}$$

We get :

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot ((g(\hat{x}) - u(\hat{x}))\nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \nabla \cdot \left((\Psi_{SL}(\Psi_0)(\hat{x}) - \Psi_{DL}(g)(\hat{x})) \nu(\hat{x}) \right) p(\hat{x}) d\Gamma_0(\hat{x}) \\
& \quad - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) \nabla \cdot (g(\hat{x})\nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& \quad - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) \{ g(\hat{y}) (\nabla_y \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) \\
& \quad \quad - g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) \\
& \quad + (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) \} d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y})
\end{aligned} \tag{A.19}$$

The terms highlighted above:

$$\begin{aligned}
& - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) (\nabla_y \nabla_y G(\hat{x}, \hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& \quad + \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) g(\hat{y}) \nabla_y G(\hat{x}, \hat{y}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& \quad - \int_{\Gamma_0} \int_{\Gamma_0} p(\hat{x}) (\nabla_y G(\hat{x}, \hat{y}) \cdot \hat{\mathbf{n}}(\hat{y})) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) d\Gamma_0(\hat{x}) d\Gamma_0(\hat{y}) \\
& = - \int_{\Gamma_0} g(\hat{y}) \left((\nabla_y \nabla_y \int_{\Gamma_0} G(\hat{x}, \hat{y}) p(\hat{x}) d\Gamma_0(\hat{x}))^T \nu(\hat{y}) \right) \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{y}) \\
& \quad + \int_{\Gamma_0} g(\hat{y}) \nabla_y \int_{\Gamma_0} p(\hat{x}) G(\hat{x}, \hat{y}) d\Gamma_0(\hat{x}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) d\Gamma_0(\hat{y}) \\
& \quad - \int_{\Gamma_0} \nabla_y \left(\int_{\Gamma_0} p(\hat{x}) G(\hat{x}, \hat{y}) d\Gamma_0(\hat{x}) \right) \cdot \hat{\mathbf{n}}(\hat{y}) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) d\Gamma_0(\hat{y}) \\
& \quad = c \int_{\Gamma_0} g(\hat{y}) (\nabla \nabla u(\hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{y}) \\
& \quad \quad - c \int_{\Gamma_0} g(\hat{y}) \nabla u(\hat{y}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) d\Gamma_0(\hat{y}) \\
& \quad \quad + c \int_{\Gamma_0} \nabla u(\hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) d\Gamma_0(\hat{y})
\end{aligned} \tag{A.20}$$

The shape gradient formula becomes:

$$\begin{aligned}
& c \int_{\Gamma_0} \Psi_0(\hat{x}) \nabla \cdot ((g(\hat{x}) - u(\hat{x}))\nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& + \int_{\Gamma_0} \nabla \cdot \left((\Psi_{SL}(\Psi_0)(\hat{x}) - \Psi_{DL}(g)(\hat{x})) \nu(\hat{x}) \right) p(\hat{x}) d\Gamma_0(\hat{x}) \\
& \quad - \frac{1}{2} \int_{\Gamma_0} p(\hat{x}) \nabla \cdot (g(\hat{x})\nu(\hat{x})) d\Gamma_0(\hat{x}) \\
& \quad + c \int_{\Gamma_0} g(\hat{y}) (\nabla \nabla u(\hat{y})^T \nu(\hat{y})) \cdot \hat{\mathbf{n}}(\hat{y}) d\Gamma_0(\hat{y}) \\
& \quad - c \int_{\Gamma_0} g(\hat{y}) \nabla u(\hat{y}) \cdot (\nabla \nu(\hat{y}) \hat{\mathbf{n}}(\hat{y})) d\Gamma_0(\hat{y}) \\
& \quad + c \int_{\Gamma_0} \nabla u(\hat{y}) \cdot \hat{\mathbf{n}}(\hat{y}) \nabla \cdot (g(\hat{y}) \nu(\hat{y})) d\Gamma_0(\hat{y})
\end{aligned} \tag{A.21}$$