ON DISCRETE SHAPE GRADIENTS OF BOUNDARY TYPE FOR PDE-CONSTRAINED SHAPE OPTIMIZATION*

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Abstract. Shape gradients have been widely used in numerical shape gradient descent algorithms for shape optimization. The two types of shape gradients, i.e., the distributed one and the boundary type, are equivalent at the continuous level but exhibit different numerical behaviors after finite element discretization. To be more specific, the boundary type shape gradient is more popular in practice due to its concise formulation and convenience to combine with shape optimization algorithms but has lower numerical accuracy. In this paper we provide a simple yet useful boundary correction for the normal derivatives of the state and adjoint equations, motivated by their continuous variational forms, to increase the accuracy and possible effectiveness of the boundary shape gradient in PDE-constrained shape optimization. We consider particularly the state equation with Dirichlet boundary conditions and provide a preliminary error estimate for the correction. Numerical results show that the corrected boundary type shape gradient has comparable accuracy to that of the distributed one. Moreover, we give a theoretical explanation for the comparable numerical accuracy of the boundary type shape gradient with that of the distributed shape gradient for Neumann boundary value problems.

Key words. Shape optimization, shape gradient, boundary formulation, boundary correction, a priori error estimate, finite element

AMS subject classifications. 49Q12, 65D15, 65K10, 65N30

1. Introduction. Shape optimization has wide applications in various fields in computational science and engineering [2, 3, 7, 17, 25, 27, 36, 39, 41]. For optimal shape design of complex systems, numerical methods and techniques are useful to find "approximate" optimal shapes with the help of computer simulations [27]. Gradient-type optimization methods are widely used shape evolution algorithms to iteratively obtain the approximate optimal domain shapes. To perform a gradient-type algorithm in shape optimization, the so-called *shape gradient*, derived from *Eulerian derivative*, is indispensable. Eulerian derivatives can be derived by *shape sensitivity analysis* [17, 28, 34, 41], which is a classic mathematical tool in shape optimization to measure the variations of an objective functional (called "*shape functional*" in shape optimization) with respect to shape variations of some domain.

Hadamard-Zolésio structure theorem [17] shows that the shape gradient for a general shape functional can be obtained by computing the Eulerian derivative in the form of a boundary integral assuming that the domain is smooth enough. Most existing research works on numerical algorithms for shape optimization rely on this structure theorem by using the boundary formulation, due to its attractive concise representation, see e.g., [11, 16, 25]. On the discrete level this type of Eulerian derivative should be discretized by, e.g., finite element method, which requires the according discretization of the state and (possible) adjoint partial differential equations (PDEs).

Finite element methods [10] are among the most popular approaches for discretizing PDEs in shape optimization (see e.g., [26]). One main reason is that the finite element method can solve PDEs on arbitrary domains and thus is flexible to domain changes in shape optimization. The accuracy of approximate shape gradients could be essential for the implementation of numerical optimization algorithms as stated in [17]. It was further pointed out in [5] that the sensitivity information needs to be very accurately computed in order for the optimization algorithms to fully converge. Recently, it is found that the finite element approximations of shape gradients in boundary formulations of Eulerian derivatives have unsatisfactory accuracy and low convergence rate with respect to the mesh size compared to those in volume formulations, see e.g., [29] for elliptic problems, [45] for eigenvalue problems, and [44] for Stokes flows. Numerical investigations even show that the approximate shape gradient flow computed with the traditional boundary formulation may fail to converge to the optimal target domain [33, 43], possibly because the poor accuracy of the approximate shape gradients does not ensure the descent property of the gradient at the discrete level. When it comes to using distributed shape gradients, i.e., the shape gradients associated with volume integrals of Eulerian derivatives in the context of numerical algorithms, we also refer to [9, 32, 40].

Aiming to enhance the accuracy of the finite element approximations of boundary type shape gradients, we propose in this paper a simple yet useful boundary correction for the normal derivatives of the state and

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adjoint equations with Dirichlet boundary conditions, motivated by their continuous variational forms. The cost of this correction requires only to inverse a boundary mass matrix for the state and adjoint state variables, respectively, and thus is negligible compared to the cost of shape gradient descent algorithm. We remark that this kind of boundary equation is extensively used to approximate Dirichlet boundary control of PDEs, see e.g., [4, 12, 15, 21, 22]. We present preliminary a priori error estimates for the finite element approximations of the boundary type shape gradients with the proposed boundary corrections. We find that the modified approximate shape gradient has higher order convergence rate and accuracy than that of the classical one, and is comparable to the distributed one when the solutions are sufficiently smooth. We believe that this kind of correction can also be used in shape optimization of parabolic equations [40], elastic structures ([3]), Stokes flows ([44]) and other related fields. On the other hand, compared to the Dirichlet case, it was observed in [29] that the boundary and distributed type shape gradients exhibit similar numerical accuracy for Neumann boundary value problems. We consider this problem and give a partial explanation for this phenomenon by a careful numerical analysis.

The remaining of this paper is organized as follows. In §2 we present a shape optimization model problem constrained by an elliptic boundary value problem. In §3, we propose a boundary correction for the normal derivatives of the state and adjoint equations with Dirichlet boundary conditions, and present a priori error estimates for the finite element approximations of shape gradients with such boundary correction. The second part of this section is devoted to an error analysis for the approximate shape gradient of boundary type for Neumann boundary value problems. For both cases we use the "non-conforming" finite elements with polygonal domain to approximate the curved domain. In §4 extensive numerical examples are presented to verify our theory.

2. Shape gradients for PDE-constrained shape optimization. Let Ω be an open bounded domain in $\mathbb{R}^n$ $(n = 2, 3)$ with Lipschitz continuous boundary $\partial\Omega$. For comparison we consider a specific example similar to the one in [29]. We are interested in the following PDE-constrained *shape functional* with $J(\cdot) : \Omega \mapsto \mathbb{R}$

$$J(\Omega) = \int_\Omega j(u)dx, \tag{2.1}$$

where $j : \mathbb{R} \to \mathbb{R}$ is C^1 and we assume further that the derivative j' is locally Lipschitz continuous (i.e., $j' \in C^{0,1}(I)$ for any compact set $I \subset \mathbb{R}$), u is the solution of the following linear elliptic state equation with either Dirichlet or Neumann boundary condition

$$\begin{cases} -\Delta u + u = f & \text{in } \Omega, \\ u = g \text{ or } \partial_{\mathbf{n}} u = g & \text{on } \Gamma := \partial\Omega, \end{cases} \tag{2.2}$$

where the functions f and g are assumed to be smooth enough which will be specified later, and they are identified with their restrictions onto Ω and $\partial\Omega$. Here $\partial_{\mathbf{n}}$ denotes the normal derivative operator with $\mathbf{n}$ being the unit outward normal on the boundary.

Throughout the paper, we make the following assumptions on the data f and g, the function $j(u)$ and the domain Ω.

ASSUMPTION 2.1.
- *$\Omega \subset \mathbb{R}^n$ is a bounded domain with a C^3 boundary $\partial\Omega$.*
- *$f \in W^{1,r}(\mathbb{R}^n)$ $(r > n)$.*
- *$g \in W^{3,r}(\mathbb{R}^n)$ $(r > n)$ for the Dirichlet case and $g \in H^2(\mathbb{R}^n)$ for the Neumann case.*
- *$j(u)$ is C^1 with its derivative j' being locally Lipschitz continuous, i.e., $j' \in C^{0,1}(I)$ for any compact set $I \subset \mathbb{R}$.*

Let us briefly introduce some basic ingredients of the velocity method [17, 41] for shape calculus. Let D $(\Omega \subset D)$ be a hold-all domain in $\mathbb{R}^n$ whose boundary ∂D is piecewise C^1. Denote

$$\begin{aligned} V^1(D) = \big\{ \boldsymbol{\mathcal{V}} \in \mathcal{D}^1(\mathbb{R}^n; \mathbb{R}^n) \mid \langle \boldsymbol{\mathcal{V}}, \mathbf{n} \rangle_{\mathbb{R}^n} = 0 \text{ on } \partial D \ \text{ except for the singular points } \bar{x} \text{ of } \partial D, \\ \boldsymbol{\mathcal{V}}(\bar{x}) = 0 \text{ for all singular points } \bar{x} \big\}. \end{aligned}$$

For a variable $t \in [0, \tau)$ with $\tau > 0$, let a vector field $\boldsymbol{\mathcal{V}} \in C\left(0, \tau; V^1(D)\right)$ and $T_t(\boldsymbol{\mathcal{V}})$ be the associated one-to-one transformation from $\bar{D}$ onto $\bar{D}$. Let $x = x(t, X)$ denote the solution to the system of ordinary differential equations

$$\frac{\mathrm{d}x}{\mathrm{d}t}(t, X) = \boldsymbol{\mathcal{V}}(t, x(t, X)), \quad x(0, X) = X. \tag{2.3}$$

Denote $\Omega_t = T_t(\boldsymbol{\mathcal{V}})(\Omega)$. The *Eulerian derivative* of $J(\Omega)$ at Ω in the direction $\boldsymbol{\mathcal{V}}$ can be expressed as the following limit

$$\mathrm{d}J(\Omega; \boldsymbol{\mathcal{V}}) := \lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t}. \tag{2.4}$$

The Eulerian derivative $\mathrm{d}J(\Omega, \boldsymbol{\mathcal{V}})$ can be formulated as an integral over the volume Ω for the so-called distributed shape gradient, as well as an integral on the boundary for the so-called boundary type shape gradient. An explicit formula for the Eulerian derivative of the shape functional $J(\Omega)$ relies on the solution p of the following adjoint problem

$$\begin{cases} -\Delta p + p = j'(u) & \text{in } \Omega, \\ p = 0 \text{ or } \partial_{\mathbf{n}} p = 0 & \text{on } \Gamma. \end{cases} \tag{2.5}$$

We summarize the known results in the following lemma dedicated to the case of Dirichlet boundary conditions.

Lemma 2.2. *Let u and p be the solutions of the primal equation (2.2) and the adjoint state equation (2.5) with Dirichlet boundary conditions, respectively. There holds*

$$\begin{aligned} \mathrm{d}J^D(\Omega, u, p; \boldsymbol{\mathcal{V}}) = \int_\Omega \Big(&\nabla u \cdot (D\boldsymbol{\mathcal{V}} + D\boldsymbol{\mathcal{V}}^T)\nabla p - f\boldsymbol{\mathcal{V}} \cdot \nabla p + \operatorname{div}\boldsymbol{\mathcal{V}}(j(u) - \nabla u \cdot \nabla p \\ &- up) + (j'(u) - p)(\nabla g \cdot \boldsymbol{\mathcal{V}}) - \nabla p \cdot \nabla(\nabla g \cdot \boldsymbol{\mathcal{V}})\Big)dx. \end{aligned} \tag{2.6}$$

The Eulerian derivative can be equivalently written as

$$\mathrm{d}J^D(\Gamma, u, p; \boldsymbol{\mathcal{V}}) = \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} \Big(j(u) + \partial_{\mathbf{n}} p \partial_{\mathbf{n}}(u - g)\Big) ds, \tag{2.7}$$

where $\boldsymbol{\mathcal{V}}_{\mathbf{n}} := \boldsymbol{\mathcal{V}} \cdot \mathbf{n}$.

Proof. For the proof we refer to [29], see also [25] and [27]. □

The distributed integral (2.6) and the boundary integral (2.7) are equivalent representations of the Eulerian derivative $\mathrm{d}J^D(\Omega, \boldsymbol{\mathcal{V}})$, and can be derived from each other by means of Gauss's theorem, see [29] for the detailed derivation. However, the formula (2.7) is more popular in the literature compared to (2.6), possibly because the boundary type admits a representative $g(\Omega)$ in the space of distributions $\mathcal{D}^k(\Gamma)$ according to the structure theorem, i.e., if Γ is smooth, there holds

$$\mathrm{d}J^D(\Gamma, u, p; \boldsymbol{\mathcal{V}}) = \langle g(\Omega), \gamma_\Gamma \boldsymbol{\mathcal{V}} \cdot \mathbf{n} \rangle_{\mathcal{D}^k(\Gamma)}, \tag{2.8}$$

where $\gamma_\Gamma \boldsymbol{\mathcal{V}} \cdot \mathbf{n}$ is the trace for the normal component of $\boldsymbol{\mathcal{V}}$ on the boundary Γ. This implies that only normal displacements of the boundary have an impact on the value of $J(\Omega)$. This expression comes in handy in many numerical methods, where the values of the velocity field $\boldsymbol{\mathcal{V}}$ on the boundary of the shape are the only ones needed.

The next result is dedicated to the case of Neumann boundary conditions.

Lemma 2.3. *[29, Remark 2.2] Let u and p be the solutions of the primal equation (2.2) and the adjoint state equation (2.5) with Neumann boundary conditions, respectively. The Eulerian derivatives read*

$$\begin{aligned} \mathrm{d}J^N(\Omega, u, p; \boldsymbol{\mathcal{V}}) = \int_\Omega \Big(&(\nabla f \cdot \boldsymbol{\mathcal{V}})p + \nabla u \cdot (D\boldsymbol{\mathcal{V}} + D\boldsymbol{\mathcal{V}}^T)\nabla p + \operatorname{div}\boldsymbol{\mathcal{V}}(fp + j(u) \\ &- \nabla u \cdot \nabla p - up)\Big)dx + \int_\Gamma (\nabla g \cdot \boldsymbol{\mathcal{V}})p + gp\operatorname{div}_\Gamma \boldsymbol{\mathcal{V}} ds, \end{aligned} \tag{2.9}$$

where $\operatorname{div}_\Gamma \boldsymbol{\mathcal{V}} := \operatorname{div}\boldsymbol{\mathcal{V}} - \mathbf{n}^T D\boldsymbol{\mathcal{V}}\mathbf{n}$ denotes the tangential divergence on Γ, and

$$\mathrm{d}J^N(\Gamma, u, p; \boldsymbol{\mathcal{V}}) = \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} \Big(j(u) - \nabla u \cdot \nabla p - up + fp + \partial_{\mathbf{n}}(gp) + Kgp\Big) ds, \tag{2.10}$$

where $K := \operatorname{div} \mathbf{n}$ is the mean curvature of Γ.

We remark that, by using the fact that

$$\nabla u = \nabla_\Gamma u + \partial_{\mathbf{n}} u \mathbf{n} = \nabla_\Gamma u + g\mathbf{n} \quad \text{and} \quad \nabla p = \nabla_\Gamma p + \partial_{\mathbf{n}} p \mathbf{n} = \nabla_\Gamma p \quad \text{on } \Gamma,$$

where one defines the tangential gradient $\nabla_\Gamma u = P \nabla u$ with $P = \mathbb{I} - \mathbf{n}\mathbf{n}^T$ and $\mathbb{I}$ being an identity matrix, we can rewrite formula (2.10) as

$$\mathrm{d}J^N(\Gamma, u, p; \boldsymbol{\mathcal{V}}) = \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} \Big(j(u) - \nabla_\Gamma u \cdot \nabla_\Gamma p - up + fp + \partial_{\mathbf{n}} gp + Kgp\Big) ds. \tag{2.11}$$

Below are a few remarks concerning the conditions in Assumption 2.1.

Remark 2.4. *In this paper we assume that $\partial\Omega$ is C^3, the reasons are as follows.*

- *As noted in Lemma 2.2, the smoothness assumption on Ω allows the derivation of the shape gradient under boundary formulation that is equivalent to the volume one.*

- *This assumption allows for higher regularity of the solutions to the state and adjoint equations which is essential for the proof of improved convergence rates of boundary shape gradients.*
- *As pointed out in [29], for the Neumann case the shape gradient has to be corrected at the corners if the boundary is only piecewise smooth. Taking Ω to be a 2D polygonal domain as example, formula (2.10) has to be corrected by adding the term (cf. [29])*

$$\sum_i p(x_i)g(x_i)\boldsymbol{\mathcal{V}}(x_i)\cdot[[\tau(x_i)]], \tag{2.12}$$

where the x_i denote the corner points and $[[\tau(x_i)]]$ is the jump of the tangential unit vector field in the corner x_i ([41, Ch. 3.8]). On the other hand, no correction has to be made to formula (2.7).
- *When the boundary Γ is only piecewise smooth, the Hadamard-Zolésio structure theorem (2.8) does not hold for the Eulerian derivatives (2.7) and (2.10) for respective Dirichlet and Neumann problems.*

When Ω is only a convex polygonal/polyhedral domain, the boundary correction can still be used, but we can not expect the same accuracy as that of the volume formulation, see Remark 3.11 for more details.

3. Discretized shape gradients for PDE-constrained shape optimization. For function spaces and norms we are going to use the notations of [1, 10]. Now we consider the finite element approximations. Let $\{\mathcal{T}_h\}_{h>0}$ be a quasi-uniform and shape regular family of triangulations of domains Ω_h approximating Ω. Define $\Gamma_h := \partial\Omega_h$. For the domain with curved boundary there are two types of finite element approximations, one is relied on the parametric finite elements (cf. [10, Section 10.4]) while the other is based on polygonal boundary approximation (cf. [8, 30]). Here we consider the latter case so that $\Omega_h \neq \Omega$, we assume further that all boundary vertices of Γ_h also lie on Γ and that at most one edge or face of a simplex belongs to Γ_h. The latter assumption is used to avoid trivial finite element solutions near the boundary for problems with homogeneous Dirichlet boundary conditions. We denote by $\langle\cdot,\cdot\rangle_\Gamma$ and $\langle\cdot,\cdot\rangle_{\Gamma_h}$ the inner products on Γ and Γ_h, respectively, associated with the norms $\|\cdot\|_{L^2(\Gamma)}$ for $L^2(\Gamma)$ and $\|\cdot\|_{L^2(\Gamma_h)}$ for $L^2(\Gamma_h)$ that are defined in the usual way. Let $(\cdot,\cdot)_h$ denote the inner product in $L^2(\Omega_h)$. Associated with $\mathcal{T}_h$ we construct the finite element space V_h which consists of piecewise polynomials of first order such that $V_h \subset H^1(\Omega_h)$. We denote by $V_h^0 := V_h \cap H_0^1(\Omega_h)$ and $V_h(\Gamma_h)$ the restriction of V_h to the boundary Γ_h. The functions in V_h^0 are globally continuous. In the following, the constants C appearing at different circumstances may be different, but are independent of h.

To deal with variational problems defined on different domains Ω_h and Ω, we need to introduce some extension operator. We define the usual Sobolev extension $E : W^{r,p}(\Omega) \to W^{r,p}(\mathbb{R}^n)$, with $r \geq 0,\ 1 \leq p \leq \infty$, satisfying $Ev|_\Omega = v$ for $v \in W^{r,p}(\Omega)$ and (cf. [8, 23, 30])

$$\|Ev\|_{W^{r,p}(\mathbb{R}^n)} \leq C\|v\|_{W^{r,p}(\Omega)}. \tag{3.1}$$

In the following, we use the same notation for a function $v \in W^{r,p}(\Omega)$ and its extension to $\mathbb{R}^n$.

3.1. Dirichlet boundary value problem. In this subsection we consider the state equation (2.2) with Dirichlet boundary condition. The variational formulation of (2.2) is to find $u \in H^1(\Omega)$ such that $u|_\Gamma = g$ and

$$(\nabla u, \nabla v) + (u, v) = (f, v) \quad \forall v \in H_0^1(\Omega). \tag{3.2}$$

On the other hand, the variational formulation of (2.5) reads: find $p \in H_0^1(\Omega)$ such that

$$(\nabla p, \nabla v) + (p, v) = (j'(u), v) \quad \forall v \in H_0^1(\Omega). \tag{3.3}$$

Now we are in the position to formulate the finite element approximations to the state and adjoint equations. For the state equation it is to find $u_h \in V_h$ such that $u_h|_{\Gamma_h} = Q_h g$ where Q_h is defined later (cf. (3.21)), and

$$(\nabla u_h, \nabla v_h)_h + (u_h, v_h)_h = (f, v_h)_h \quad \forall v_h \in V_h^0. \tag{3.4}$$

For the discretization of the adjoint state equation it is to find $p_h \in V_h^0$ such that

$$(\nabla p_h, \nabla v_h)_h + (p_h, v_h)_h = (j'(u_h), v_h)_h \quad \forall v_h \in V_h^0. \tag{3.5}$$

We remark that the right hand sides of (3.4) and (3.5) are usually evaluated by quadrature formulas. However, in the current paper we do not consider the quadrature errors but we only focus on the finite element discretization errors. Then we have the error estimates [8, Theorem 1]

$$\begin{aligned} \|u - u_h\|_{L^2(\Omega_h)} + h\|u - u_h\|_{H^1(\Omega_h)} &\leq Ch^2(\|f\|_{L^2(\Omega)} + \|g\|_{H^2(\Omega)}), \\ \|p - p_h\|_{L^2(\Omega_h)} + h\|p - p_h\|_{H^1(\Omega_h)} &\leq Ch^2(\|j'(u)\|_{L^2(\Omega)} + \|f\|_{L^2(\Omega)} + \|g\|_{H^2(\Omega)}). \end{aligned} \tag{3.6}$$

The following stability estimates also hold

$$\|u_h\|_{H^1(\Omega_h)} \leq C(\|f\|_{L^2(\Omega)} + \|g\|_{H^1(\Omega)}), \quad \|p_h\|_{H^1(\Omega_h)} \leq C(\|j'(u)\|_{L^2(\Omega)} + \|f\|_{L^2(\Omega)} + \|g\|_{H^1(\Omega)}). \tag{3.7}$$

Moreover, we assume the following $W^{1,\infty}$-norm error estimate

$$\|u-u_h\|_{W^{1,\infty}(\Omega_h)}+\|p-p_h\|_{W^{1,\infty}(\Omega_h)}\le Ch(\|u\|_{W^{2,\infty}(\Omega)}+\|p\|_{W^{2,\infty}(\Omega)}). \tag{3.8}$$

REMARK 3.1. *The L^2-norm and H^1-norm error estimates (3.6) have been proved in [8, Theorem 1] in the two-dimensional case. However, it is possible to extend the results to the three-dimensional case, because all the necessary geometric errors for the approximation of a three-dimensional curved domain by a polygonal domain have already been proved in [30, 31], see for instance, Section 2.2 of [30]. A different proof for the estimates (3.6) from that of [8] can be found in [15] for both 2D and 3D curved domains.*

REMARK 3.2. *The $W^{1,\infty}$-norm error estimate (3.8) for the finite element approximation of the solution to an elliptic equation with Dirichlet boundary condition based on boundary polygonal approximation is not precisely available in the literature. However, we can find in [30] such an error estimate for the corresponding Neumann boundary value problem. We expect that the methods of proof in [30] can be applied to elliptic Dirichlet problem to derive (3.8). This is partially confirmed by a private communication with Professor Tomoya Kemmochi. In the special case that Ω is convex so that $\Omega_h\subset\Omega$, the equations (2.2) and (2.5) also hold in Ω_h, we can expect that the standard $W^{1,\infty}$-norm error estimate (cf. [10, Chapter 8]) for elliptic Dirichlet problems implies (3.8).*

REMARK 3.3. *Since (3.5) is not a direct Galerkin approximation to (3.3), in order to derive the error estimates (3.6) and (3.8) involving p we have to introduce the intermediate discrete quantity $p_h(u)\in V_h^0$ such that*

$$(\nabla p_h(u),\nabla v_h)_h+(p_h(u),v_h)_h=(j'(u),v_h)_h\quad\forall v_h\in V_h^0.$$

Now $p_h(u)$ is the standard Galerkin discretization of p and the following error estimates hold

$$\begin{aligned}\|p-p_h(u)\|_{L^2(\Omega_h)}+h\|p-p_h(u)\|_{H^1(\Omega_h)}&\le Ch^2\|j'(u)\|_{L^2(\Omega)},\\ \|p-p_h(u)\|_{W^{1,\infty}(\Omega_h)}&\le Ch\|p\|_{W^{2,\infty}(\Omega)}.\end{aligned}$$

By using the triangle inequality we only need to estimate

$$\begin{aligned}\|p_h(u)-p_h\|_{L^2(\Omega_h)}+\|p_h(u)-p_h\|_{H^1(\Omega_h)}&\le C\|j'(u)-j'(u_h)\|_{L^2(\Omega_h)}\le C\|j'\|_{C^{0,1}(I)}\|u-u_h\|_{L^2(\Omega_h)},\\ \|p_h(u)-p_h\|_{W^{1,\infty}(\Omega_h)}&\le C\|j'(u)-j'(u_h)\|_{L^\infty(\Omega_h)}\le C\|j'\|_{C^{0,1}(I)}\|u-u_h\|_{L^\infty(\Omega_h)},\end{aligned}$$

where we used the stability (3.7) and Theorem 8.5.3 in [10]. Here $I:=[\underline{u},\bar{u}]$, $\underline{u}$ and $\bar{u}$ are chosen such that $-\infty<\underline{u}\le u(x),u_h(x)\le\bar{u}<\infty$ in Ω_h and j' is bounded on I, we refer to [29, pp. 468, eq. (3.20)] for more details. Combining the above estimates we can derive the error estimates for the adjoint state equation.

With the discrete state u_h and adjoint state p_h at hand, the discretized boundary type Eulerian derivative for the shape optimization problem reads

$$\mathrm{d}_hJ^D(\Gamma_h,u_h,p_h;\boldsymbol{\mathcal{V}})=\int_{\Gamma_h}\boldsymbol{\mathcal{V}}_{\mathbf{n}_h}\Big(j(u_h)+\partial_{\mathbf{n}_h}p_h(\partial_{\mathbf{n}_h}u_h-\partial_{\mathbf{n}_h}g\Big)ds. \tag{3.9}$$

This approach is extensively used in the literature as it is easy to implement. In [29] the authors compared the numerical performance of two discretized shape gradients, one with a volumetric formulation while the other with a boundary formulation. It is claimed that the volume type discrete shape gradient has better approximation property for state equations with Dirichlet boundary condition compared to the counterpart boundary integrals, which is then confirmed by extensive numerical examples (cf. [29, Section 4]).

PROPOSITION 3.1. *[35, Theorem 2.2.4 and 2.2.9] Let u_h and p_h be Ritz-Galerkin linear Lagrange finite element approximations of the solutions u and p of (2.2) and (2.5) associated with the Dirichlet boundary conditions. Assume that $f\in H^1(\mathbb{R}^n)$, $g\in H^3(\mathbb{R}^n)$, $\Gamma_h=\Gamma$, and that there holds*

$$\|u\|_{W^{2,q}(\Omega)}\le C_q\|f\|_{L^\infty(\Omega)}\qquad\textit{for all } 1<q<\infty,$$

where $C_q\sim\frac{1}{q-1}$ for $q\to 1$ and $C_q\sim q$ for $q\to\infty$ (cf. [20, Theorem 9.8 and 9.9]). We remark that the above $W^{2,q}$-elliptic regularity holds if $\partial\Omega\in C^{1,1}$, $f\in L^q(\Omega)$ and $g\in W^{2,q}(\Omega)$ (cf. [23, Theorem 2.4.2.5]). Then

$$\left|\mathrm{d}J^D(\Gamma,u,p;\boldsymbol{\mathcal{V}})-\mathrm{d}_hJ^D(\Gamma,u_h,p_h;\boldsymbol{\mathcal{V}})\right|\le Ch|\log h|\|\boldsymbol{\mathcal{V}}\cdot\mathbf{n}\|_{L^\infty(\partial\Omega)}.$$

Moreover, for the discrete shape gradient of the volume type we have

$$\left|\mathrm{d}J^D(\Omega,u,p;\boldsymbol{\mathcal{V}})-\mathrm{d}_hJ^D(\Omega,u_h,p_h;\boldsymbol{\mathcal{V}})\right|\le Ch^2\|\boldsymbol{\mathcal{V}}\|_{W^{2,4}(\Omega)}.$$

In this paper we propose a modified discrete shape gradient on Γ_h:

$$\tilde{\mathrm{d}}_hJ^D(\Gamma_h,u_h,p_h;\boldsymbol{\mathcal{V}})=\int_{\Gamma_h}\boldsymbol{\mathcal{V}}_{\mathbf{n}}\circ a_h\Big(j(u_h)+\partial^h_{\mathbf{n}_h}p_h(\partial^h_{\mathbf{n}_h}u_h-\partial_{\mathbf{n}}g\circ a_h)\Big)ds_h, \tag{3.10}$$

where a_h is defined as in (3.15), $\partial^h_{\mathbf{n}_h} u_h \in V_h(\Gamma_h)$ and $\partial^h_{\mathbf{n}_h} p_h \in V_h(\Gamma_h)$ solve the following discrete variational problems:

$$\langle \partial^h_{\mathbf{n}_h} u_h, v_h \rangle_{\Gamma_h} = (\nabla u_h, \nabla v_h)_h + (u_h, v_h)_h - (f, v_h)_h \quad \forall v_h \in V_h \tag{3.11}$$

and

$$\langle \partial^h_{\mathbf{n}_h} p_h, v_h \rangle_{\Gamma_h} = (\nabla p_h, \nabla v_h)_h + (p_h, v_h)_h - (j'(u_h), v_h)_h \quad \forall v_h \in V_h. \tag{3.12}$$

We remark that an additional work in the modified discrete shape gradient (3.10) is paid to the solution of two boundary equations (3.11) and (3.12), which only requires the solution of linear systems with small numbers of degrees of freedom are required to be solved. Moreover, the evaluation of the right-hand sides in (3.11) and (3.12) is only performed in the neighboring elements of the boundary nodes because of the discrete state equation (3.4) and adjoint equation (3.5).

Remark 3.4. *Note that in the classical approximation (3.9) one has one order loss for the approximations $\partial_{\mathbf{n}_h} u_h$ of $\partial_{\mathbf{n}} u$, this is because we use Optimize-then-Discretize approach ([5]) for the optimization problem, i.e., we derive the first order optimality system and the Eulerian derivative of the objective functional at the continuous level. Then we discretize the optimality system and define the discrete shape gradient at the discrete level by inserting the discrete state and adjoint state. While for the modified scheme (3.10), the approximations $\partial^h_{\mathbf{n}_h} u_h$ and $\partial^h_{\mathbf{n}_h} p_h$ have the same polynomial degree as that of u_h and p_h, thus these corrections mimick the procedure of Discretize-then-Optimize approach by using discrete counterparts of integration by parts. Moreover, compared to the classical discrete shape gradient (3.9) which is discontinuous when $\mathbb{P}_1$ Lagrange finite elements are used for u_h and p_h, our modified formula is continuous on the boundary, and thus can be used for continuous extensions in the shape optimization algorithms (cf. [11]).*

Remark 3.5. *Instead of the boundary polygonal approximation Ω_h of Ω utilized in the present paper, we can also use the isoparametric finite element method to solve partial differential equations posed on curved domain (cf. [10, Section 10.4]). This is particularly useful if we try to use higher order finite element methods. In this case, we can expect a better boundary approximation Γ_h to Γ than the polygonal approximation, along with a better outward normal approximation $\mathbf{n}_h$ to $\mathbf{n}$. Therefore, we can also define the modified shape gradient (3.10) based on the recovered solutions to (3.11) and (3.12) defined on Γ_h. The following analysis can be carried over to the isoparametric finite element approximation, but a rigorous justification is still necessary.*

In the following we will show in Theorem 3.10 that the modified discrete shape gradient (3.10) has improved convergence rate compared to the classical one (3.9). The proof relies on an improved approximation property of $\partial^h_{\mathbf{n}_h} u_h$ to $\partial_{\mathbf{n}} u$ and $\partial^h_{\mathbf{n}_h} p_h$ to $\partial_{\mathbf{n}} p$, presented in Lemma 3.8, compared to that of $\partial_{\mathbf{n}_h} p_h$ and $\partial_{\mathbf{n}_h} u_h$. Also we need to introduce an auxiliary problem (cf. eq. (3.43)) and use a duality argument to improve the convergence rate, compared to the approach of Theorem 3.2 in [29].

Before giving the main results we present some preliminary results. Firstly, it follows that for each $u \in H^{\frac{3}{2}+\varepsilon}(\Omega)$ $(\varepsilon > 0)$ we can define the outward normal trace $\partial_{\mathbf{n}} u \in L^2(\Gamma)$ for a Lipschitz domain Ω (cf. [23, Theorem 1.5.1.2]). Let $u \in H^1(\Omega)$ be the solution to the elliptic equation (2.2) with $f \in L^2(\mathbb{R}^n)$ and $g \in H^2(\mathbb{R}^n)$, we conclude that $u \in \{u \in H^1(\Omega) : -\Delta u + u \in L^2(\Omega)\} \subset H^{\frac{3}{2}+\varepsilon}(\Omega)$ for some $\varepsilon \in (0, \frac{1}{2}]$ if Ω is a Lipschitz polygonal domain (cf. [24], Theorem 2.4.3 for the two-dimensional case and Corollary 2.6.7 for the three-dimensional case). In addition, there holds $\partial_{\mathbf{n}} u \in H^{\varepsilon}(\Gamma)$ and this quantity satisfies (cf. [6, Theorem 3.2])

$$\langle \partial_{\mathbf{n}} u, v \rangle_{\Gamma} = (\nabla u, \nabla v) + (u, v) - (f, v) \quad \forall v \in H^1(\Omega). \tag{3.13}$$

Under Assumption 2.1, we have for each $f \in W^{1,r}(\Omega)$, $g \in W^{3,r}(\Omega)$ $(r > n)$ that $u \in W^{3,r}(\Omega)$ (cf. [15]), and thus $u \in W^{2,\infty}(\Omega)$ by the Sobolev embedding theorem (cf. [1]) and $\partial_{\mathbf{n}} u \in H^{\frac{3}{2}}(\Gamma)$ by the trace theorem (cf. [23, Section 1.5.1]).

Similarly, we have the variational problem for the outward normal derivative of the solution to the adjoint equation

$$\langle \partial_{\mathbf{n}} p, v \rangle_{\Gamma} = (\nabla p, \nabla v) + (p, v) - (j'(u), v) \quad \forall v \in H^1(\Omega). \tag{3.14}$$

The above regularity results also hold for the adjoint problem under the regularity assumption that $j'(u) \in W^{1,r}(\Omega)$ $(r > n)$.

In the following we present some results on the approximation property between Ω_h and Ω. Note that with the boundary polygonal approximation we have $\Omega_h \neq \Omega$. We define the projection $a_h : \Gamma_h \to \Gamma$ as (cf. [14], [8, 13] for 2D and [30, 42] for 3D)

$$a_h(x) := x + \delta_h(x)\mathbf{n}_h(x) \quad \text{for } x \in e \subset \Gamma_h, \tag{3.15}$$

where $\mathbf{n}_h$ is the constant normal to Γ_h on e and $\delta_h(x)$ (which could be negative) is chosen in such a way that $a_h(x) \in \Gamma$ (cf. Figure 3.1 for an illustration in 2D). Then it can be shown that a_h is locally bijective for

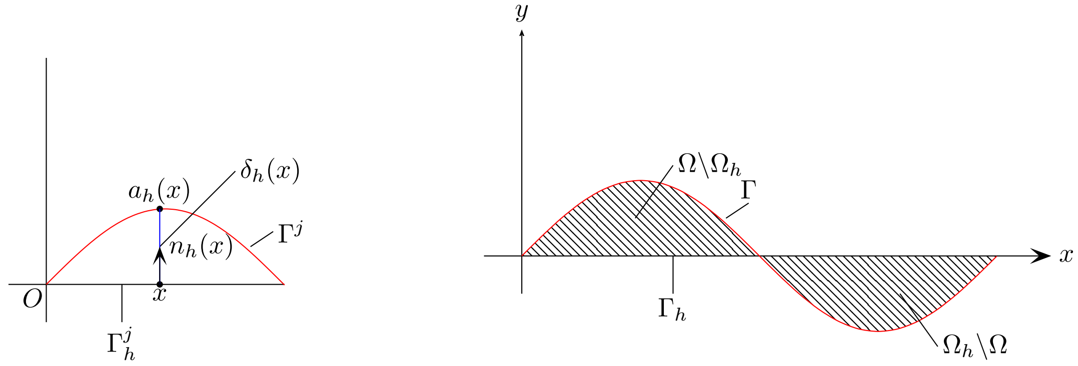

FIG. 3.1. *An illustration of the mapping a_h (left) and the approximation Ω_h to Ω (right).*

sufficiently small h and $\text{dist}(\Gamma, \Gamma_h) \le Ch^2$, $|\Omega\backslash\Omega_h| \le Ch^2$, $|\Omega_h\backslash\Omega| \le Ch^2$ (cf. [8, 30]). Furthermore, for any $v \in L^2(\Gamma_h)$ we have ([15, 13, 31])

$$\int_{\Gamma_h} v ds_h = \int_{\Gamma} v \circ a_h^{-1} t_h ds, \quad \text{with } t_h = \frac{ds_h}{ds}, \tag{3.16}$$

where ds and ds_h denote the smooth and discrete surface measures, respectively.

The above derivation implies the following error estimate (cf. [13, eq. (4.3)] for 2D and [30, eq. (2.1)], [31, Section 8] for 3D)

$$\left| \int_{\Gamma} v ds - \int_{\Gamma_h} v \circ a_h ds_h \right| \le Ch^2 \int_{\Gamma} |v| ds \quad \forall v \in L^1(\Gamma) \tag{3.17}$$

and the stability (cf. [8, eq. (2.5)] for 2D and [31, Section 8] for 3D)

$$\frac{1}{C}\|v\|_{L^2(\Gamma)} \le \|v \circ a_h\|_{L^2(\Gamma_h)} \le C\|v\|_{L^2(\Gamma)} \quad \forall v \in L^2(\Gamma). \tag{3.18}$$

On the other hand, we associate with V_h an analogous space $\tilde{V}_h$ in Ω. To do so we follow the ideas of [8] where the 2D case was considered, and extend the results to 3D. For each $v_h \in V_h$ we denote by $\tilde{v}_h : \bar{\Omega} \to \mathbb{R}$ as follows: if Ω_e is the subset of $\Omega\backslash\Omega_h$ bounded by the boundary face $e \subset T \cap \Gamma_h$ and the curved surface $\tilde{e} \subset \partial\Omega$, $\tilde{v}_h|_{\Omega_e}$ is defined as the linear extension of v_h from T. That is, for any $v_h|_T := \sum_{i=1}^{n+1} v_i^T \phi_i^T(x)$, where ϕ_i^T denotes the nodal basis function associated with the nodal x_i of T and v_i^T is the nodal value of v_h at x_i, we define $\tilde{v}_h|_{\Omega_e} := \sum_{i=1}^{n+1} v_i^T \phi_i^T(x)$ for any $x \in \Omega_e$. Then we define

$$\tilde{V}_h := \{\tilde{v}_h : \ v_h \in V_h\}$$

and there holds (cf. [8, eq. (2.6)] and [30, Section 2.3])

$$\|\tilde{v}_h\|_{H^1(\Omega)} \le C\|v_h\|_{H^1(\Omega_h)}. \tag{3.19}$$

On Γ we can define the discrete piecewise linear finite element space

$$\hat{V}_h := \{v_h \circ a_h^{-1} : \ v_h \in V_h(\Gamma_h)\}.$$

With this definition we remark that for $v_h \in V_h$ the identity $\tilde{v}_h|_\Gamma = v_h|_{\Gamma_h} \circ a_h^{-1}$ is not necessarily valid, but there holds the following estimate.

LEMMA 3.6. *For each $v_h \in V_h$ let $\tilde{v}_h$ be its linear extension to Ω defined above. Then there holds*

$$\|\tilde{v}_h - v_h \circ a_h^{-1}\|_{L^2(\Gamma)} \le Ch^{\frac{3}{2}}\|\nabla v_h\|_{L^2(\Omega_h)}. \tag{3.20}$$

Proof. In fact, it follows from (3.18) and Taylor's expansion that

$$\begin{aligned}
\|\tilde{v}_h - v_h \circ a_h^{-1}\|^2_{L^2(\Gamma)} &\leq C\|\tilde{v}_h \circ a_h - v_h\|^2_{L^2(\Gamma_h)} \\
&= C \sum_{e\subset\Gamma_h, e\subset\partial T} \int_e \Big(\sum_{i=1}^{n+1} v_i^T \left(\phi_i^T(a_h(x)) - \phi_i^T(x)\right)\Big)^2 ds \\
&= C \sum_{e\subset\Gamma_h, e\subset\partial T} \int_e \Big(\sum_{i=1}^{n+1} v_i^T \nabla\phi_i^T(x)\cdot(a_h(x) - x)\Big)^2 ds \\
&\leq Ch^4 \sum_{e\subset\Gamma_h, e\subset\partial T} \int_e \Big| \sum_{i=1}^{n+1} v_i^T \nabla\phi_i^T\Big|^2 ds \\
&= Ch^4 \|\nabla v_h\|^2_{L^2(\Gamma_h)} \\
&\leq Ch^3 \sum_{T\in\mathcal{T}_h} \int_T \Big| \sum_{i=1}^{n+1} v_i^T \nabla\phi_i^T\Big|^2 dx \\
&= Ch^3 \|\nabla v_h\|^2_{L^2(\Omega_h)},
\end{aligned}$$

where we used the facts that $|a_h(x) - x| \leq Ch^2$ (cf. [8, Section 2] and [30, Section 2.2]) and

$$\int_e \Big| \sum_{i=1}^{n+1} v_i^T \nabla\phi_i^T\Big|^2 ds \leq Ch^{-1} \int_T \Big| \sum_{i=1}^{n+1} v_i^T \nabla\phi_i^T\Big|^2 dx$$

when T is an element with face e, because $\nabla\phi_i^T$ is a constant on each element T. ◻

Now we can define some projection operators. Firstly, we consider the L^2-projection operator $Q_h : L^2(\Gamma_h) \to V_h(\Gamma_h)$ defined by:

$$\langle Q_h v, v_h\rangle_{\Gamma_h} = \langle v, v_h\rangle_{\Gamma_h} \quad \forall v_h \in V_h(\Gamma_h). \tag{3.21}$$

Similarly, we can define the L^2-projection operator $\hat{Q}_h : L^2(\Gamma) \to \hat{V}_h$ such that for any $v \in L^2(\Gamma)$ there holds

$$\langle v, \tilde{v}_h\rangle_\Gamma = \langle \hat{Q}_h v, \tilde{v}_h\rangle_\Gamma \quad \forall \tilde{v}_h \in \hat{V}_h. \tag{3.22}$$

According to [8, eq. (2.20)] one has

$$\|(I - \hat{Q}_h)v\|_{L^2(\Gamma)} \leq Ch^s|v|_{H^s(\Gamma)}, \quad 0 \leq s \leq 2. \tag{3.23}$$

Note that $Q_h(v\circ a_h) \neq (\hat{Q}_h v)\circ a_h$ for $v \in L^2(\Gamma)$, but we have the following approximation result (cf. [8, Lemma 4])

$$\begin{aligned}
\|Q_h(v\circ a_h)\circ a_h^{-1} - \hat{Q}_h v\|_{L^2(\Gamma)} &\leq C\|Q_h(v\circ a_h) - (\hat{Q}_h v)\circ a_h\|_{L^2(\Gamma_h)} \\
&\leq Ch^2\|v\|_{L^2(\Gamma)}.
\end{aligned} \tag{3.24}$$

Remark 3.7. *The error estimate (3.23) for the $L^2(\Gamma)$ projection $\hat{Q}_h$ is proved in [8] for 2D case. However, with a closer look at the proof we find that only the approximation property of the finite element space $\hat{V}_h$ and the stability of the projection $\hat{Q}_h$ are used. Therefore, the extension to 3D is possible. For a slightly different definition of the projection $\hat{Q}_h$ in both 2D and 3D we refer to [15, eq. (3.7) and (3.8)]. Moreover, (3.24) is also proved in [8, Lemma 4] for 2D, and the proof relies only on the mapping property (3.16) and the fact $|1 - t_h| \leq Ch^2$ which are also valid in 3D. Therefore, the estimate (3.24) holds also in the 3D case.*

Converting the boundary formula (3.10) to Γ we have

$$\tilde{\mathrm{d}}_h J^D(\Gamma, u_h, p_h; \boldsymbol{\mathcal{V}}) = \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}}\Big(j(u_h\circ a_h^{-1}) + \widehat{\partial^h_{\mathbf{n}_h} p_h}(\widehat{\partial^h_{\mathbf{n}_h} u_h} - \partial_{\mathbf{n}} g)\Big)t_h ds, \tag{3.25}$$

where $\widehat{\partial^h_{\mathbf{n}_h} u_h} := \partial^h_{\mathbf{n}_h} u_h \circ a_h^{-1}$ and $\widehat{\partial^h_{\mathbf{n}_h} p_h} := \partial^h_{\mathbf{n}_h} p_h \circ a_h^{-1}$, $t_h := \frac{ds_h}{ds}$ with ds and ds_h denoting the smooth and discrete surface measures, respectively (cf. (3.16)). We remark that in the above formula (3.10) we use $\boldsymbol{\mathcal{V}}_{\mathbf{n}} \circ a_h$ instead of $\boldsymbol{\mathcal{V}}\cdot\mathbf{n}_h$, because for the latter case we have one order lost when we convert the integral on Γ_h to that on Γ, since one can only expect $|\mathbf{n}_h \circ a_h^{-1} - \mathbf{n}| \leq Ch$ (cf. [13, eq. (4.1)] and [31, Section 8]).

Before proving the main result we first investigate the approximation property of $\partial^h_{\mathbf{n}_h} u_h$ to $\partial_{\mathbf{n}} u$ and $\partial^h_{\mathbf{n}_h} p_h$ to $\partial_{\mathbf{n}} p$.

Lemma 3.8. *Let $\partial_{\mathbf{n}} u$ and $\partial_{\mathbf{n}} p$ be the continuous outward normal derivatives defined in (3.13) and (3.14), respectively. Let $\partial^h_{\mathbf{n}_h} u_h$ and $\partial^h_{\mathbf{n}_h} p_h$ be the approximations defined in (3.11) and (3.12), respectively. Assume that*

Assumption 2.1 holds. Then we have

$$\begin{aligned} \|\partial_{\mathbf{n}} u - \widehat{\partial^h_{\mathbf{n}_h} u_h}\|_{L^2(\Gamma)} &\le Ch(\|u\|_{W^{3,r}(\Omega)} + \|f\|_{H^1(\Omega)}), \\ \|\partial_{\mathbf{n}} p - \widehat{\partial^h_{\mathbf{n}_h} p_h}\|_{L^2(\Gamma)} &\le Ch(\|u\|_{W^{3,r}(\Omega)} + \|f\|_{H^1(\Omega)} + \|p\|_{W^{3,r}(\Omega)}) \end{aligned} \tag{3.26}$$

for some $r > n$.

Proof. We first estimate $\|\partial_{\mathbf{n}} u - \widehat{\partial^h_{\mathbf{n}_h} u_h}\|_{L^2(\Gamma)}$. Note that by the triangle inequality

$$\|\partial_{\mathbf{n}} u - \widehat{\partial^h_{\mathbf{n}_h} u_h}\|_{L^2(\Gamma)} \le \|\partial_{\mathbf{n}} u - \hat{Q}_h \partial_{\mathbf{n}} u\|_{L^2(\Gamma)} + \|\hat{Q}_h \partial_{\mathbf{n}} u - \widehat{\partial^h_{\mathbf{n}_h} u_h}\|_{L^2(\Gamma)}. \tag{3.27}$$

Now the proof can be divided into the following steps.

Step 1: For the first term, it follows from the standard projection error estimate (3.23) that

$$\|\partial_{\mathbf{n}} u - \hat{Q}_h \partial_{\mathbf{n}} u\|_{L^2(\Gamma)} \le Ch\|\partial_{\mathbf{n}} u\|_{H^1(\Gamma)} \le Ch\|u\|_{H^{5/2}(\Omega)}. \tag{3.28}$$

Step 2: Now it remains to estimate the second term $\|\hat{Q}_h \partial_{\mathbf{n}} u - \widehat{\partial^h_{\mathbf{n}_h} u_h}\|_{L^2(\Gamma)}$. This step can be further divided into the following several steps.

Substep 2.1: To begin with, we first derive the error equation for $\partial_{\mathbf{n}} u - \widehat{\partial^h_{\mathbf{n}_h} u_h}$. For each $\xi_h \in V_h(\Gamma_h)$ let $S_h\xi_h$ be an extension of ξ_h into Ω_h such that $S_h\xi_h \in V_h$, $S_h\xi_h = \xi_h$ on Γ_h and satisfies

$$(\nabla S_h\xi_h, \nabla v_h)_h + (S_h\xi_h, v_h)_h = 0 \quad \forall v_h \in V_h^0. \tag{3.29}$$

We denote by $\mathring{S}_h\xi_h \in V_h$ the extension of ξ_h to the interior of the domain Ω_h by setting $\mathring{S}_h\xi_h = 0$ at the interior nodes of the triangulation. By using the norm equivalence in finite-dimensional spaces we have for any $q \in [1, \infty)$ (cf. [4, eq. (29)] and [21, Lemma 5.3]):

$$\|\mathring{S}_h\xi_h\|_{L^q(\Omega_h)} + h\|\nabla \mathring{S}_h\xi_h\|_{L^q(\Omega_h)} \le Ch^{\frac{1}{q}}\|\xi_h\|_{L^q(\Gamma_h)}. \tag{3.30}$$

Note that for any $\xi_h \in V_h(\Gamma_h)$ there holds

$$\begin{aligned} \langle \partial^h_{\mathbf{n}_h} u_h, \xi_h\rangle_{\Gamma_h} &= (\nabla u_h, \nabla S_h\xi_h)_h + (u_h, S_h\xi_h)_h - (f, S_h\xi_h)_h \\ &= (\nabla u_h, \nabla \mathring{S}_h\xi_h)_h + (u_h, \mathring{S}_h\xi_h)_h - (f, \mathring{S}_h\xi_h)_h \end{aligned}$$

by recalling the definition (3.11).

On the other hand, (3.11) is equivalent to

$$\langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h\rangle_\Gamma = (\nabla u_h, \nabla v_h)_h + (u_h, v_h)_h - (f, v_h)_h + \langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h - v_h \circ a_h^{-1} t_h\rangle_\Gamma \quad \forall v_h \in V_h \tag{3.31}$$

by using (3.16) and the fact that $\langle \partial^h_{\mathbf{n}_h} u_h, v_h\rangle_{\Gamma_h} = \langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, v_h \circ a_h^{-1} t_h\rangle_\Gamma$. Denote by $v_h = \mathring{S}_h\xi_h$ and its linear extension by $\tilde{v}_h = \widetilde{\mathring{S}_h\xi_h}$. Then we obtain from (3.13) and (3.31) the error equation for $\partial_{\mathbf{n}} u - \widehat{\partial^h_{\mathbf{n}_h} u_h}$:

$$\begin{aligned} \langle \partial_{\mathbf{n}} u - \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h\rangle_\Gamma =& (\nabla u, \nabla \tilde{v}_h) + (u, \tilde{v}_h) - (f, \tilde{v}_h) - \langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h - \xi_h \circ a_h^{-1} t_h\rangle_\Gamma \\ & - (\nabla u_h, \nabla v_h)_h - (u_h, v_h)_h + (f, v_h)_h \\ =& (\nabla(u - u_h), \nabla v_h)_h + (u - u_h, v_h)_h - \langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h - \xi_h \circ a_h^{-1} t_h\rangle_\Gamma + M_h(u, \tilde{v}_h), \end{aligned} \tag{3.32}$$

where

$$M_h(u, \tilde{v}_h) = \int_{\Omega\setminus\Omega_h} (\nabla u \cdot \nabla \tilde{v}_h + u\tilde{v}_h - f\tilde{v}_h)dx - \int_{\Omega_h\setminus\Omega} (\nabla u \cdot \nabla v_h + uv_h - fv_h)dx.$$

Substep 2.2: Then, we give some estimates for the last two terms on the right-hand side of the above identity (3.32). The remaining term $(\nabla(u - u_h), \nabla v_h)_h + (u - u_h, v_h)_h$ will be estimated in *Step 3*. Using $|1 - t_h| \le Ch^2$, (3.18), Lemma 3.6 and (3.30) we have

$$\begin{aligned} |\langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h - v_h \circ a_h^{-1} t_h\rangle_\Gamma| &\le |\langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h - v_h \circ a_h^{-1}\rangle_\Gamma| + |\langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, v_h \circ a_h^{-1}(1 - t_h)\rangle_\Gamma| \\ &\le C\|\partial^h_{\mathbf{n}_h} u_h\|_{L^2(\Gamma_h)}(\|\tilde{v}_h \circ a_h - v_h\|_{L^2(\Gamma_h)} + h^2\|v_h\|_{L^2(\Gamma_h)}) \\ &\le C\|\partial^h_{\mathbf{n}_h} u_h\|_{L^2(\Gamma_h)}(h^{\frac{3}{2}}\|\nabla v_h\|_{L^2(\Omega_h)} + h^2\|v_h\|_{L^2(\Gamma_h)}) \\ &\le Ch\|\partial^h_{\mathbf{n}_h} u_h\|_{L^2(\Gamma_h)}\|v_h\|_{L^2(\Gamma_h)}. \end{aligned} \tag{3.33}$$

Now it remains to estimate $M_h(u, \tilde{v}_h)$. Using [8, Lemma 2] or [30, eq. (2.1)] we have for $v \in H^1(\Omega)$

$$\|v\|_{L^2(\Omega\backslash\Omega_h)} \le C(h\|v\|_{L^2(\Gamma)} + h^2\|\nabla v\|_{L^2(\Omega)}) \le Ch\|v\|_{H^1(\Omega)}. \tag{3.34}$$

This combined with (3.18), (3.19), Lemma 3.6 implies that for any $v_h \in V_h$,

$$\begin{aligned}
\|\tilde{v}_h\|_{L^2(\Omega\backslash\Omega_h)} &\le C(h\|\tilde{v}_h\|_{L^2(\Gamma)} + h^2\|\nabla\tilde{v}_h\|_{L^2(\Omega)}) \\
&\le C(h\|\tilde{v}_h - v_h \circ a_h^{-1}\|_{L^2(\Gamma)} + h\|v_h \circ a_h^{-1}\|_{L^2(\Gamma)} + h^2\|\nabla\tilde{v}_h\|_{L^2(\Omega)}) \\
&\le C(h\|v_h\|_{L^2(\Gamma_h)} + h^2\|\nabla v_h\|_{L^2(\Omega_h)}).
\end{aligned}$$

Assume that $\bar{\Omega}\backslash\Omega_h = \sum_i \bar{\Omega}_h^i$ where Ω_h^i is the curved region bounded by $\Gamma_h^i \subset \Gamma_h$ and $\Gamma^i \subset \Gamma$. For the readers' convenience, we first recall some known estimates for functions near the boundary region, presented in [8, eq. (2.9)] for the 2D case:

$$\|\varphi\|^2_{L^2(\Omega_h^i)} \le C\left(h^2\|\varphi\|^2_{L^2(\Gamma^i)} + h^4\left\|\frac{\partial\varphi}{\partial x_2}\right\|^2_{L^2(\Omega_h^i)}\right),$$

where to illustrate the idea a special piece Γ_h^i is chosen as $\Gamma_h^i = \{(x_1, x_2) : x_2 = 0,\ 0 \le x_1 < C_1 h\}$ so that $\Gamma^i = \{(x_1, x_2) : x_2 = \delta_h(x_1) \ge 0,\ 0 \le x_1 < C_1 h\}$, see also Lemma 2 and Lemma 3 in [8] for the general case. A similar result is presented in [30, eq. (2.1)] for 2D and 3D cases:

$$\|f\|_{L^s(\Gamma(\delta))} \le C(\delta^{1/s}\|f\|_{L^s(\Gamma)} + \delta\|\nabla f\|_{L^s(\Gamma(\delta))}), \quad s \in [1, \infty],$$

where $\Gamma(\delta)$ denotes the tubular neighborhood of Γ with distance δ that is the so-called boundary skin. Now we can derive using the above results that

$$\|\nabla\tilde{v}_h\|_{L^2(\Omega_h^i)} \le C\Big(h\|\nabla\tilde{v}_h\|_{L^2(\Gamma^i)} + h^2\|\nabla\tilde{v}_h\|_{L^2(\Omega_h^i)}\Big),$$

where we used the fact that $\tilde{v}_h$ is a linear polynomial in Ω_h^i so that $\|\nabla\tilde{v}_h\|_{H^1(\Omega_h^i)} = \|\nabla\tilde{v}_h\|_{L^2(\Omega_h^i)}$. That is, for h sufficiently small, the second term on the right-hand side of the above inequality can be absorbed by the left-hand side. Then, we obtain from the fact that $\nabla\tilde{v}_h$ in the curved region Ω_h^i is exactly the same piecewise constant vector as ∇v_h in the boundary element related to Γ_h^i and (3.18)

$$\begin{aligned}
\|\nabla\tilde{v}_h\|_{L^2(\Omega\backslash\Omega_h)} \le Ch\|\nabla\tilde{v}_h\|_{L^2(\Gamma)} &= Ch\Big(\sum_i \|\nabla\tilde{v}_h\|^2_{L^2(\Gamma^i)}\Big)^{\frac{1}{2}} \\
&\le Ch\Big(\sum_i \|\nabla v_h\|^2_{L^2(\Gamma_h^i)}\Big)^{\frac{1}{2}} \\
&= Ch\|\nabla v_h\|_{L^2(\Gamma_h)} \le C\|v_h\|_{L^2(\Gamma_h)},
\end{aligned}$$

where the standard inverse estimate has been used in the last inequality above. Recalling $v_h = \mathring{S}_h\xi_h$, the above estimates combined with (3.30) with $q = 2$ imply that

$$\begin{aligned}
&\int_{\Omega\backslash\Omega_h} (\nabla u \cdot \nabla\tilde{v}_h + u\tilde{v}_h - f\tilde{v}_h)dx \\
&\le \|\nabla u\|_{L^2(\Omega\backslash\Omega_h)}\|\nabla\tilde{v}_h\|_{L^2(\Omega\backslash\Omega_h)} + \Big|\int_{\Omega\backslash\Omega_h} (u - f)\tilde{v}_h dx\Big| \\
&\le C|\Omega\backslash\Omega_h|^{\frac{1}{2}}\|u\|_{W^{1,\infty}(\Omega)}\|\nabla\tilde{v}_h\|_{L^2(\Omega\backslash\Omega_h)} + Ch^2(\|u\|_{H^1(\Omega)} + \|f\|_{H^1(\Omega)})(\|v_h\|_{L^2(\Gamma_h)} + h\|\nabla v_h\|_{L^2(\Omega_h)}) \\
&\le Ch\|u\|_{W^{1,\infty}(\Omega)}\|v_h\|_{L^2(\Gamma_h)} + Ch^2(\|u\|_{H^1(\Omega)} + \|f\|_{H^1(\Omega)})\|v_h\|_{L^2(\Gamma_h)} \\
&\le Ch(\|u\|_{W^{1,\infty}(\Omega)} + h\|u\|_{H^1(\Omega)} + h\|f\|_{H^1(\Omega)})\|v_h\|_{L^2(\Gamma_h)}.
\end{aligned} \tag{3.35}$$

Similarly, using [8, Lemma 3] or [30, eq. (2.2)] we have for $v \in H^1(\Omega_h)$

$$\|v\|_{L^2(\Omega_h\backslash\Omega)} \le C(h\|v\|_{L^2(\Gamma_h)} + h^2\|\nabla v\|_{L^2(\Omega_h)}) \le Ch\|v\|_{H^1(\Omega_h)}. \tag{3.36}$$

This implies that for any $v_h \in V_h \subset H^1(\Omega_h)$,

$$\|v_h\|_{L^2(\Omega_h\backslash\Omega)} \le C(h\|v_h\|_{L^2(\Gamma_h)} + h^2\|\nabla v_h\|_{L^2(\Omega_h)}).$$

With abuse of notation, we assume again that $\bar{\Omega}_h\backslash\Omega = \sum_i \bar{\Omega}_h^i$ where Ω_h^i is the curved region bounded by $\Gamma_h^i \subset \Gamma_h$ and $\Gamma^i \subset \Gamma$. Similar to the above estimates, it follows from [8, eq. (2.10)] or [30, eq. (2.2)] that

$$\|\nabla v_h\|_{L^2(\Omega_h^i)} \le C\Big(h\|\nabla v_h\|_{L^2(\Gamma_h^i)} + h^2\|\nabla v_h\|_{L^2(\Omega_h^i)}\Big),$$

therefore,

$$\|\nabla v_h\|_{L^2(\Omega_h\backslash\Omega)} \le Ch\|\nabla v_h\|_{L^2(\Gamma_h)} \le C\|v_h\|_{L^2(\Gamma_h)}.$$

Recalling again $v_h = \mathring{S}_h\xi_h$ and using (3.30) with $q=2$, we are now ready to prove that

$$\begin{aligned}
&\int_{\Omega_h\backslash\Omega}(\nabla u\cdot\nabla v_h + uv_h - fv_h)dx \\
&\le \|\nabla u\|_{L^2(\Omega_h\backslash\Omega)}\|\nabla v_h\|_{L^2(\Omega_h\backslash\Omega)} + \Big|\int_{\Omega_h\backslash\Omega}(u-f)v_h dx\Big| \\
&\le C|\Omega_h\backslash\Omega|^{\frac12}\|u\|_{W^{1,\infty}(\Omega_h)}\|\nabla v_h\|_{L^2(\Omega_h\backslash\Omega)} + Ch^2(\|u\|_{H^1(\Omega_h)}+\|f\|_{H^1(\Omega_h)})(\|v_h\|_{L^2(\Gamma_h)} + h\|\nabla v_h\|_{L^2(\Omega_h)}) \\
&\le Ch\|u\|_{W^{1,\infty}(\Omega)}\|v_h\|_{L^2(\Gamma_h)} + Ch^2(\|u\|_{H^1(\Omega)}+\|f\|_{H^1(\Omega)})(\|v_h\|_{L^2(\Gamma_h)} + h\|\nabla v_h\|_{L^2(\Omega_h)}) \\
&\le Ch(\|u\|_{W^{1,\infty}(\Omega)}+\|f\|_{H^1(\Omega)})\|v_h\|_{L^2(\Gamma_h)},
\end{aligned} \tag{3.37}$$

where we have used (3.1) because u has been continuously extended from Ω to $\Omega_h\backslash\Omega$. Combining the estimates (3.35) and (3.37) we obtain that

$$M_h(u,\tilde v_h) \le Ch(\|u\|_{W^{1,\infty}(\Omega)}+\|f\|_{H^1(\Omega)})\|v_h\|_{L^2(\Gamma_h)}. \tag{3.38}$$

Step 3: Finally, we turn to the estimate of the second term in (3.27). Let $z_h\in V_h$ be the solution to the following discrete variational problem

$$z_h|_{\Gamma_h} = \hat Q_h(\partial_{\mathbf n}u)\circ a_h - \partial^h_{\mathbf n_h}u_h \quad\text{and}\quad (\nabla z_h,\nabla v_h)_h + (z_h,v_h)_h = 0 \quad \forall v_h\in V_h^0. \tag{3.39}$$

That is, $z_h := S_h(\hat Q_h(\partial_{\mathbf n}u)\circ a_h - \partial^h_{\mathbf n_h}u_h)$. Further, we define $\bar z_h := \mathring{S}_h(\hat Q_h(\partial_{\mathbf n}u)\circ a_h - \partial^h_{\mathbf n_h}u_h)$ and $\tilde{\bar z}_h$ as its linear extension to Ω.

Using the definition of $\hat Q_h$ we have

$$\begin{aligned}
\|\hat Q_h\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|^2_{L^2(\Gamma)} &= \langle\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}, \hat Q_h\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\rangle_\Gamma \\
&= \langle\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}, \tilde{\bar z}_h\rangle_\Gamma + \langle\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}, \hat Q_h\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h} - \tilde{\bar z}_h\rangle_\Gamma \\
&=: I_1 + I_2.
\end{aligned}$$

For the first term I_1 we use the error equation (3.32) by setting $\tilde v_h := \tilde{\bar z}_h$. We conclude from (3.18), (3.33), (3.38), the L^2 error estimate (3.6) and the $W^{1,\infty}$ error estimate (3.8) that

$$\begin{aligned}
\langle\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}, \tilde{\bar z}_h\rangle_\Gamma =& (\nabla(u-u_h),\nabla\bar z_h)_h + (u-u_h,\bar z_h)_h - \langle\widehat{\partial^h_{\mathbf n_h}u_h}, \tilde{\bar z}_h - \bar z_h\circ a_h^{-1}t_h\rangle_\Gamma + M_h(u,\tilde{\bar z}_h) \\
\le& \|\nabla(u-u_h)\|_{L^\infty(\Omega_h)}\|\nabla\bar z_h\|_{L^1(\Omega_h)} + \|u-u_h\|_{L^2(\Omega_h)}\|\bar z_h\|_{L^2(\Omega_h)} \\
&- \langle\widehat{\partial^h_{\mathbf n_h}u_h}, \tilde{\bar z}_h - \bar z_h\circ a_h^{-1}t_h\rangle_\Gamma + M_h(u,\tilde{\bar z}_h) \\
\le& C(h\|u\|_{W^{2,\infty}(\Omega)} + h^2\|u\|_{H^2(\Omega)})\|\hat Q_h(\partial_{\mathbf n}u)\circ a_h - \partial^h_{\mathbf n_h}u_h\|_{L^2(\Gamma_h)} \\
&+ Ch\|\partial^h_{\mathbf n_h}u_h\|_{L^2(\Gamma_h)}\|\bar z_h\|_{L^2(\Gamma_h)} + Ch(\|u\|_{W^{1,\infty}(\Omega)}+\|f\|_{H^1(\Omega)})\|\bar z_h\|_{L^2(\Gamma_h)} \\
\le& Ch(\|u\|_{W^{2,\infty}(\Omega)} + \|\partial^h_{\mathbf n_h}u_h\|_{L^2(\Gamma_h)} + \|f\|_{H^1(\Omega)})\|\hat Q_h\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|_{L^2(\Gamma)},
\end{aligned}$$

where in the second last step we used (3.30) with $q=1$ and the embedding $L^2(\Gamma_h)\hookrightarrow L^1(\Gamma_h)$. For the second term I_2 the estimates (3.18), Lemma 3.6 and (3.30) yield

$$\begin{aligned}
\langle\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}, \hat Q_h\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h} - \tilde{\bar z}_h\rangle_\Gamma &= \langle\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}, \bar z_h\circ a_h^{-1} - \tilde{\bar z}_h\rangle_\Gamma \\
&\le \|\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|_{L^2(\Gamma)}\|\bar z_h\circ a_h^{-1} - \tilde{\bar z}_h\|_{L^2(\Gamma)} \\
&\le Ch^{\frac32}\|\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|_{L^2(\Gamma)}\|\nabla\bar z_h\|_{L^2(\Omega_h)} \\
&\le Ch\|\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|_{L^2(\Gamma)}\|\hat Q_h\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|_{L^2(\Gamma)}.
\end{aligned}$$

This implies that

$$\begin{aligned}
\|\hat Q_h\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|_{L^2(\Gamma)} &\le Ch(\|u\|_{W^{2,\infty}(\Omega)} + \|\partial^h_{\mathbf n_h}u_h\|_{L^2(\Gamma_h)} + \|f\|_{H^1(\Omega)} + \|\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|_{L^2(\Gamma)}) \\
&\le Ch(\|u\|_{W^{2,\infty}(\Omega)} + \|\partial^h_{\mathbf n_h}u_h\|_{L^2(\Gamma_h)} + \|f\|_{H^1(\Omega)} + \|\partial_{\mathbf n}u\|_{L^2(\Gamma)}).
\end{aligned} \tag{3.40}$$

Combining (3.28) and (3.40) we complete the estimate of $\|\partial_{\mathbf n}u - \widehat{\partial^h_{\mathbf n_h}u_h}\|_{L^2(\Gamma)}$.

The estimate for $\|\partial_{\mathbf{n}}p - \widehat{\partial^h_{\mathbf{n}_h} p_h}\|_{L^2(\Gamma)}$ can be proved in a similar way. For any $\xi_h \in V_h(\Gamma_h)$ we still denote by $v_h = \mathring{S}_h \xi_h$ and its linear extension by $\tilde{v}_h = \widetilde{\mathring{S}_h \xi_h}$. We obtain from (3.14) and (3.12) the error equation for $\partial_{\mathbf{n}}p - \widehat{\partial^h_{\mathbf{n}_h} p_h}$:

$$
\begin{aligned}
\langle \partial_{\mathbf{n}}p - \widehat{\partial^h_{\mathbf{n}_h} p_h}, \tilde{v}_h\rangle_\Gamma =&(\nabla p, \nabla \tilde{v}_h) + (p, \tilde{v}_h) - (j'(u), \tilde{v}_h) - (\nabla p_h, \nabla v_h)_h - (p_h, v_h)_h \\
&+ (j'(u_h), v_h)_h - \langle \widehat{\partial^h_{\mathbf{n}_h} p_h}, \tilde{v}_h - \xi_h \circ a_h^{-1} t_h\rangle_\Gamma \\
=&(j'(u_h) - j'(u), v_h)_h + (\nabla(p - p_h), \nabla v_h)_h + (p - p_h, v_h)_h \\
&- \langle \widehat{\partial^h_{\mathbf{n}_h} p_h}, \tilde{v}_h - \xi_h \circ a_h^{-1} t_h\rangle_\Gamma + N_h(p, \tilde{v}_h),
\end{aligned}
\tag{3.41}
$$

where

$$
N_h(p, \tilde{v}_h) = \int_{\Omega\setminus\Omega_h} (\nabla p \cdot \nabla \tilde{v}_h + p\tilde{v}_h - j'(u)\tilde{v}_h)dx - \int_{\Omega_h\setminus\Omega} (\nabla p \cdot \nabla v_h + p v_h - j'(u) v_h)dx.
$$

A similar error estimate for $\langle \widehat{\partial^h_{\mathbf{n}_h} p_h}, \tilde{v}_h - \xi_h \circ a_h^{-1} t_h\rangle_\Gamma$ and $N_h(p, \tilde{v}_h)$ can be derived as in (3.33) and (3.38), respectively. The remaining estimates are very similar as above, except for the following term which can be estimated as

$$
\begin{aligned}
(j'(u_h) - j'(u), v_h)_h &\le \|j'(u) - j'(u_h)\|_{L^2(\Omega_h)} \|v_h\|_{L^2(\Omega_h)} \\
&\le C\|j'\|_{C^{0,1}(I)} \|u - u_h\|_{L^2(\Omega_h)} h^{\frac{1}{2}} \|\xi_h\|_{L^2(\Gamma_h)} \\
&\le C h^{\frac{5}{2}} \|u\|_{H^2(\Omega)} \|\xi_h\|_{L^2(\Gamma_h)}
\end{aligned}
\tag{3.42}
$$

by considering (3.6) and (3.30). Then we finish the proof. ◻

Remark 3.9. *There is another way to prove Lemma 3.8 by avoiding the $W^{1,\infty}$-norm error estimate (3.8) for finite element approximation to elliptic equation with Dirichlet boundary condition, but using instead the $W^{1,\infty}$-norm error estimate for Lagrange interpolation (cf. [15, Theorem 4.1]). In this case we use the extension operator S_h instead of $\mathring{S}_h$ and define the error equation (3.32) in Ω.*

To illustrate the main idea we follow the notations in [15, Section 3]. For each element $T \in \mathcal{T}_h$ there exists an affine and bijective mapping

$$
F_T : \hat{T} \subset \mathbb{R}^n \to T \subset \mathbb{R}^n, \quad F_T(\hat{x}) = A_T \hat{x} + b_T,
$$

for a fixed reference element $\hat{T}$. We denote by $\tilde{\mathcal{T}}_h$ an exact triangulation of Ω, which can be constructed by replacing the boundary element of $\mathcal{T}_h$ with curved elements. For each $T \in \mathcal{T}_h$ there exists a mapping $\Phi_T \in C^3(\hat{T}, \mathbb{R}^n)$ such that $\tilde{F}_T := F_T + \Phi_T$ maps $\hat{T}$ onto a curved n-simplex $\tilde{T} \in \tilde{\mathcal{T}}_h$. Then we can define the mapping G_h locally by $G_h|_T := \tilde{F}_T \circ F_T^{-1}$ such that it is a homeomorphism between Ω_h and Ω.

Now for any function $u_h \in V_h$ we extend it to Ω, denoting by $\tilde{u}_h$ this extension, by composing u_h with the mapping function $G_h : \Omega_h \to \Omega$ (cf. [15, Section 3]), i.e., $\tilde{u}_h = u_h \circ G_h^{-1}$. Define $\tilde{V}_h := \{\tilde{v}_h : \ v_h \in V_h\}$. For any $\xi_h \in V_h(\Gamma_h)$ we denote by $v_h = S_h \xi_h$ and by $\tilde{v}_h$ its extension. Let I_h be the Lagrange interpolation operator corresponding to V_h, we denote by $\tilde{I}_h : C^0(\bar{\Omega}) \to \tilde{V}_h$ the Lagrange interpolation operator associated with $\tilde{V}_h$, such that $(\tilde{I}_h u) \circ G_h = I_h(u \circ G_h)$ on Γ_h (cf. [15, p. 2802]).

Analogously to the derivation of (3.32), we obtain by using the definition of S_h that

$$
\begin{aligned}
\langle \partial_{\mathbf{n}}u - \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h\rangle_\Gamma =&(\nabla u, \nabla \tilde{v}_h) + (u, \tilde{v}_h) - (f, \tilde{v}_h) - \langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h - \xi_h \circ G_h^{-1} t_h\rangle_\Gamma \\
&- (\nabla u_h, \nabla v_h)_h - (u_h, v_h)_h + (f, v_h)_h \\
=&(\nabla u, \nabla \tilde{v}_h) + (u, \tilde{v}_h) - (f, \tilde{v}_h) - \langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h - \xi_h \circ G_h^{-1} t_h\rangle_\Gamma \\
&- (\nabla \tilde{I}_h u, \nabla v_h)_h - (\tilde{I}_h u, v_h)_h + (f, v_h)_h \\
=&(\nabla(u - \tilde{I}_h u), \nabla \tilde{v}_h) + (u - \tilde{I}_h u, \tilde{v}_h) \\
&- \langle \widehat{\partial^h_{\mathbf{n}_h} u_h}, \tilde{v}_h - \xi_h \circ G_h^{-1} t_h\rangle_\Gamma + M_h(\tilde{I}_h u, \tilde{v}_h),
\end{aligned}
$$

where

$$
M_h(\tilde{I}_h u, \tilde{v}_h) = \int_{\Omega\setminus\Omega_h} (\nabla \tilde{I}_h u \cdot \nabla \tilde{v}_h + \tilde{I}_h u \tilde{v}_h - f\tilde{v}_h)dx - \int_{\Omega_h\setminus\Omega} (\nabla \tilde{I}_h u \cdot \nabla v_h + \tilde{I}_h u v_h - f v_h)dx.
$$

The last two terms can be estimated in the conventional way, cf. [15, eq. (3.4)] for the estimate of $M_h(\tilde{I}_h u, \tilde{v}_h)$ and (3.33) for the estimate of the second last term. Following the arguments of [15, eq. (4.9)] and using the $W^{1,\infty}$-norm error estimate for the Lagrange interpolation $\tilde{I}_h u$, the main difference is the following estimate *(compare with the $W^{1,\infty}(\Omega_h)$ error estimate for $u-u_h$ and the $W^{1,1}(\Omega_h)$ error estimate for $\bar z_h$ in Step 3 of the proof of Lemma 3.8)*

$$
\begin{aligned}
(\nabla(u-\tilde I_h u),\nabla\tilde v_h)+(u-\tilde I_h u,\tilde v_h) &\le C\Big(\int_\Omega \omega^{-1}|\nabla(u-\tilde I_h u)|^2\Big)^{\frac12}\Big(\int_\Omega \omega|\nabla\tilde v_h|^2\Big)^{\frac12}+\|u-\tilde I_h u\|_{L^2(\Omega)}\|\tilde v_h\|_{L^2(\Omega)}\\
&\le Ch\|u\|_{W^{2,\infty}(\Omega)}\Big(\int_\Omega \omega^{-1}\Big)^{\frac12}\|\tilde v_h\|_{L^2(\Gamma)}+Ch^2\|\tilde v_h\|_{L^2(\Gamma)}\\
&\le Ch\sqrt{|\log h|}\|\tilde v_h\|_{L^2(\Gamma)},
\end{aligned}
$$

where ω is defined as in [15, Lemma 3.2] and we used the following estimate in [15, Lemma 3.2]

$$
\int_\Omega (\|\tilde v_h\|^2+\omega|\nabla\tilde v_h|^2)\le C\|\xi_h\|_{L^2(\Gamma_h)}.
$$

The above error estimate could be used in the proof of Lemma 3.8 with v_h replaced by z_h defined in (3.39). Then we could expect a similar result to Lemma 3.8 with convergence order $O(h\sqrt{|\log h|})$.

Now we are ready to prove our main result in this subsection.

THEOREM 3.10. *Let u and p be the continuous solutions to the state equation (2.2) and the adjoint equation (2.5) with Dirichlet boundary conditions, while u_h and p_h denote the discrete solutions to (3.4) and (3.5), respectively. Assume that Assumption 2.1 holds. Then we have*

$$
|\mathrm{d}J^D(\Gamma,u,p;\boldsymbol{\mathcal{V}})-\tilde{\mathrm{d}}_hJ^D(\Gamma,u_h,p_h;\boldsymbol{\mathcal{V}})|\le Ch^2(\|u\|_{W^{3,r}(\Omega)}+\|f\|_{H^1(\Omega)}+\|g\|_{H^3(\Omega)}+\|p\|_{W^{3,r}(\Omega)})^2\|\boldsymbol{\mathcal{V}}_{\mathbf n}\|_{H^{3/2}(\Gamma)}
$$

for some $r>n$.

Proof. Recalling the definitions of $\mathrm{d}J^D(\Gamma,u,p;\boldsymbol{\mathcal{V}})$ in (2.7) and $\tilde{\mathrm{d}}_hJ^D(\Gamma,u_h,p_h;\boldsymbol{\mathcal{V}})$ in (3.25), we have

$$
\begin{aligned}
\mathrm{d}J^D(\Gamma,u,p;\boldsymbol{\mathcal{V}})-\tilde{\mathrm{d}}_hJ^D(\Gamma,u_h,p_h;\boldsymbol{\mathcal{V}}) &= \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf n}\Big[j(u)-j(u_h\circ a_h^{-1})+\partial_{\mathbf n}p(\partial_{\mathbf n}u-\partial_{\mathbf n}g)-\widehat{\partial^h_{\mathbf n_h}p_h}(\widehat{\partial^h_{\mathbf n_h}u_h}-\partial_{\mathbf n}g)\Big]ds\\
&\quad+\int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf n}\Big[j(u_h\circ a_h^{-1})+\widehat{\partial^h_{\mathbf n_h}p_h}(\widehat{\partial^h_{\mathbf n_h}u_h}-\partial_{\mathbf n}g)\Big](1-t_h)ds\\
&=:J_1+J_2.
\end{aligned}
$$

It is easy to verify that

$$
|J_2|\le Ch^2(\|u\|_{H^2(\Omega)}+\|p\|_{H^2(\Omega)}+\|f\|_{L^2(\Omega)}+\|g\|_{H^2(\Omega)})
$$

because $|1-t_h|\le Ch^2$. Now we estimate J_1. The first and second terms of J_1 can be estimated as follows by using (3.23), the stability of $\hat Q_h$ and (3.24):

$$
\begin{aligned}
\int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf n}(j(u)-j(u_h\circ a_h^{-1}))ds &\le \|\boldsymbol{\mathcal{V}}_{\mathbf n}\|_{L^2(\Gamma)}\|j(u)-j(u_h\circ a_h^{-1})\|_{L^2(\Gamma)}\\
&\le C\|\boldsymbol{\mathcal{V}}_{\mathbf n}\|_{L^2(\Gamma)}\|j\|_{C^{0,1}(I)}\|u-u_h\circ a_h^{-1}\|_{L^2(\Gamma)}\\
&= C\|\boldsymbol{\mathcal{V}}_{\mathbf n}\|_{L^2(\Gamma)}\|j\|_{C^{0,1}(I)}\|g|_\Gamma-Q_h(g|_{\Gamma_h})\circ a_h^{-1}\|_{L^2(\Gamma)}\\
&\le C\|\boldsymbol{\mathcal{V}}_{\mathbf n}\|_{L^2(\Gamma)}\|j\|_{C^{0,1}(I)}(\|g|_\Gamma-\hat Q_h(g|_\Gamma)\|_{L^2(\Gamma)}+\|\hat Q_h(g|_\Gamma)-\hat Q_h(g|_{\Gamma_h}\circ a_h^{-1})\|_{L^2(\Gamma)}\\
&\quad+\|\hat Q_h(g|_{\Gamma_h}\circ a_h^{-1})-Q_h(g|_{\Gamma_h})\circ a_h^{-1}\|_{L^2(\Gamma)})\\
&\le C\|\boldsymbol{\mathcal{V}}_{\mathbf n}\|_{L^2(\Gamma)}\|j\|_{C^{0,1}(I)}(h^2\|g\|_{H^2(\Gamma)}+\|g|_\Gamma-g|_{\Gamma_h}\circ a_h^{-1}\|_{L^2(\Gamma)}+h^2\|g\|_{H^2(\Gamma)})\\
&\le Ch^2\|\boldsymbol{\mathcal{V}}_{\mathbf n}\|_{L^2(\Gamma)}\|j\|_{C^{0,1}(I)}\|g\|_{H^3(\Omega)},
\end{aligned}
$$

where we used [8, Lemma 1] or [30, eq. (2.1)] in the last step to estimate $\|g|_\Gamma-g|_{\Gamma_h}\circ a_h^{-1}\|_{L^2(\Gamma)}$. For the remaining terms we have

$$
\begin{aligned}
\boldsymbol{\mathcal{V}}_{\mathbf n}\big[\partial_{\mathbf n}p(\partial_{\mathbf n}u-\partial_{\mathbf n}g)-\widehat{\partial^h_{\mathbf n_h}p_h}(\widehat{\partial^h_{\mathbf n_h}u_h}-\partial_{\mathbf n}g)\big] =&\boldsymbol{\mathcal{V}}_{\mathbf n}\big[\partial_{\mathbf n}p(\partial_{\mathbf n}u-\widehat{\partial^h_{\mathbf n_h}u_h})+(\partial_{\mathbf n}p-\widehat{\partial^h_{\mathbf n_h}p_h})\partial_{\mathbf n}u\\
&-(\partial_{\mathbf n}p-\widehat{\partial^h_{\mathbf n_h}p_h})\partial_{\mathbf n}g-(\partial_{\mathbf n}p-\widehat{\partial^h_{\mathbf n_h}p_h})(\partial_{\mathbf n}u-\widehat{\partial^h_{\mathbf n_h}u_h})\big].
\end{aligned}
$$

Let w be the solution to the following problem

$$
\begin{cases}
-\Delta w+w=0 & \text{in } \Omega\\
w=\boldsymbol{\mathcal{V}}_{\mathbf n}\partial_{\mathbf n}p & \text{on } \Gamma.
\end{cases}
\tag{3.43}
$$

The variational formulation is to find $w\in H^1(\Omega)$ and $w=\boldsymbol{\mathcal{V}}_{\mathbf n}\partial_{\mathbf n}p$ on Γ such that

$$
(\nabla w,\nabla v)+(w,v)=0\quad \forall v\in H^1_0(\Omega),
\tag{3.44}
$$

while its finite element approximation can be written as: find $w_h \in V_h$ such that

$$(\nabla w_h, \nabla v_h)_h + (w_h, v_h)_h = 0 \quad \forall v_h \in V_h^0, \quad w_h = Q_h(\boldsymbol{\mathcal{V}}_{\mathbf{n}} \partial_{\mathbf{n}} p \circ a_h) \text{ on } \Gamma_h. \tag{3.45}$$

Since $p \in H^3(\Omega) \cap H_0^1(\Omega)$, we have $\partial_{\mathbf{n}} p \in H^{\frac{3}{2}}(\Gamma)$ by the trace theorem (cf. [23, Section 1.5.1]) and thus $\boldsymbol{\mathcal{V}}_{\mathbf{n}} \partial_{\mathbf{n}} p \in H^{\frac{3}{2}}(\Gamma)$ if $\boldsymbol{\mathcal{V}}$ is sufficiently smooth, this implies $w \in H^2(\Omega)$. Then it follows from Theorem 1 in [8] and Remark 3.1 that

$$\|w - w_h\|_{H^1(\Omega_h)} \le Ch^{s-\frac{1}{2}} \|\boldsymbol{\mathcal{V}}_{\mathbf{n}} \partial_{\mathbf{n}} p\|_{H^s(\Gamma)}, \quad \frac{1}{2} \le s \le \frac{3}{2}. \tag{3.46}$$

Denote by $\tilde{w}_h$ the linear extension of w_h to Ω. Firstly, we have

$$\begin{aligned}
\langle \boldsymbol{\mathcal{V}}_{\mathbf{n}} \partial_{\mathbf{n}} p, \partial_{\mathbf{n}} u - \widehat{\partial_{\mathbf{n}_h}^h u_h} \rangle_\Gamma =& \langle \boldsymbol{\mathcal{V}}_{\mathbf{n}} \partial_{\mathbf{n}} p - \tilde{w}_h, \partial_{\mathbf{n}} u - \widehat{\partial_{\mathbf{n}_h}^h u_h} \rangle_\Gamma + \langle \tilde{w}_h, \partial_{\mathbf{n}} u - \widehat{\partial_{\mathbf{n}_h}^h u_h} \rangle_\Gamma \\
=& \langle \boldsymbol{\mathcal{V}}_{\mathbf{n}} \partial_{\mathbf{n}} p - \tilde{w}_h, \partial_{\mathbf{n}} u - \widehat{\partial_{\mathbf{n}_h}^h u_h} \rangle_\Gamma - \langle \widehat{\partial_{\mathbf{n}_h}^h u_h}, \tilde{w}_h - w_h \circ a_h^{-1} t_h \rangle_\Gamma \\
&+ (\nabla(u - u_h), \nabla w_h)_h + (u - u_h, w_h)_h + M_h(u, \tilde{w}_h) \\
=& \langle \boldsymbol{\mathcal{V}}_{\mathbf{n}} \partial_{\mathbf{n}} p - \tilde{w}_h, \partial_{\mathbf{n}} u - \widehat{\partial_{\mathbf{n}_h}^h u_h} \rangle_\Gamma - \langle \widehat{\partial_{\mathbf{n}_h}^h u_h}, \tilde{w}_h - w_h \circ a_h^{-1} t_h \rangle_\Gamma \\
&+ (\nabla(u - u_h), \nabla(w_h - w))_h + (u - u_h, w_h - w)_h + \langle u - u_h, \partial_{\mathbf{n}_h} w \rangle_{\Gamma_h} \\
&+ M_h(u, \tilde{w}_h) + (-\Delta w + w, u - u_h)_{\Omega_h \setminus \Omega},
\end{aligned} \tag{3.47}$$

where (3.43) is used in the last equality by testing $u - u_h$ and integration by parts on Ω_h. In fact, by using (3.43) we have

$$\begin{aligned}
0 &= (-\Delta w + w, u - u_h)_{\Omega_h \cap \Omega} \\
&= (-\Delta w + w, u - u_h)_h - (-\Delta w + w, u - u_h)_{\Omega_h \setminus \Omega} \\
&= (\nabla w, \nabla(u - u_h))_h + (w, u - u_h)_h - \langle \partial_{\mathbf{n}_h} w, u - u_h \rangle_{\Gamma_h} - (-\Delta w + w, u - u_h)_{\Omega_h \setminus \Omega}
\end{aligned}$$

by using the fact that w, u have been extended to $\Omega_h \setminus \Omega$.

Now it remains to estimate the right-hand side of (3.47) terms by terms. An application of (3.6) and (3.46) yields

$$\begin{aligned}
(\nabla(u - u_h), \nabla(w_h - w))_h + (u - u_h, w_h - w)_h &\le \|u - u_h\|_{H^1(\Omega_h)} \|w - w_h\|_{H^1(\Omega_h)} \\
&\le Ch^2 (\|f\|_{L^2(\Omega)} + \|g\|_{H^2(\Omega)}) \|\boldsymbol{\mathcal{V}}_{\mathbf{n}} \partial_{\mathbf{n}} p\|_{H^{\frac{3}{2}}(\Gamma)}.
\end{aligned} \tag{3.48}$$

On the other hand, using (3.6) we obtain

$$(-\Delta w + w, u - u_h)_{\Omega_h \setminus \Omega} \le \|w\|_{H^2(\Omega_h)} \|u - u_h\|_{L^2(\Omega_h)} \le Ch^2 \|u\|_{H^2(\Omega)} \|w\|_{H^2(\Omega)}. \tag{3.49}$$

A direct use of (3.33) gives only first order convergence for $\langle \widehat{\partial_{\mathbf{n}_h}^h u_h}, \tilde{w}_h - w_h \circ a_h^{-1} t_h \rangle_\Gamma$. However, proceeding as in (3.33) and taking into account the proof of Lemma 3.6 give

$$\begin{aligned}
|\langle \widehat{\partial_{\mathbf{n}_h}^h u_h}, \tilde{w}_h - w_h \circ a_h^{-1} t_h \rangle_\Gamma| &\le |\langle \widehat{\partial_{\mathbf{n}_h}^h u_h}, \tilde{w}_h - w_h \circ a_h^{-1} \rangle_\Gamma| + |\langle \widehat{\partial_{\mathbf{n}_h}^h u_h}, w_h \circ a_h^{-1} (1 - t_h) \rangle_\Gamma| \\
&\le C \|\partial_{\mathbf{n}_h}^h u_h\|_{L^2(\Gamma_h)} (\|\tilde{w}_h \circ a_h - w_h\|_{L^2(\Gamma_h)} + h^2 \|w_h\|_{L^2(\Gamma_h)}) \\
&\le C \|\partial_{\mathbf{n}_h}^h u_h\|_{L^2(\Gamma_h)} (h^2 \|\nabla w_h\|_{L^2(\Gamma_h)} + h^2 \|w_h\|_{L^2(\Gamma_h)}) \\
&\le C \|\partial_{\mathbf{n}_h}^h u_h\|_{L^2(\Gamma_h)} (h^2 \|\nabla \tilde{w}_h\|_{L^2((\Omega \setminus \Omega_h) \cup (\Omega_h \setminus \Omega))} + h^2 \|w_h\|_{L^2(\Gamma_h)}) \\
&\le Ch^2 \|\partial_{\mathbf{n}_h}^h u_h\|_{L^2(\Gamma_h)} \|w_h\|_{H^1(\Omega_h)},
\end{aligned} \tag{3.50}$$

where we have used the third last inequality in the proof of Lemma 3.6, the trace inequality

$$\|\nabla w_h\|_{L^2(\Gamma_h^i)} \le C \|\nabla \tilde{w}_h\|_{L^2(\Omega_h^i)}^{\frac{1}{2}} \|\nabla \tilde{w}_h\|_{H^1(\Omega_h^i)}^{\frac{1}{2}} \le C \|\nabla \tilde{w}_h\|_{L^2(\Omega_h^i)}$$

and the fact that $\tilde{w}_h$ is linear in Ω_h^i, while in this case we assume $(\bar{\Omega} \setminus \Omega_h) \cup (\bar{\Omega}_h \setminus \Omega) = \sum_i \bar{\Omega}_h^i$ such that Ω_h^i is the curved region bounded by $\Gamma_h^i \subset \Gamma_h$ and $\Gamma^i \subset \Gamma$. Similarly, a careful calculation implies

$$\begin{aligned}
M_h(u, \tilde{w}_h) =& \int_{\Omega \setminus \Omega_h} (\nabla u \cdot \nabla \tilde{w}_h + u \tilde{w}_h - f \tilde{w}_h) dx - \int_{\Omega_h \setminus \Omega} (\nabla u \cdot \nabla w_h + u w_h - f w_h) dx \\
\le& \|\nabla u\|_{L^2(\Omega \setminus \Omega_h)} (\|\nabla(\tilde{w}_h - w)\|_{L^2(\Omega \setminus \Omega_h)} + \|\nabla w\|_{L^2(\Omega \setminus \Omega_h)}) + \left| \int_{\Omega \setminus \Omega_h} (u - f) \tilde{w}_h dx \right| \\
&+ \|\nabla u\|_{L^2(\Omega_h \setminus \Omega)} (\|\nabla(w_h - w)\|_{L^2(\Omega_h \setminus \Omega)} + \|\nabla w\|_{L^2(\Omega_h \setminus \Omega)}) + \left| \int_{\Omega_h \setminus \Omega} (u - f) w_h dx \right| \\
\le& Ch| \|u\|_{H^2(\Omega)} (h \|w\|_{H^2(\Omega)} + h \|w\|_{H^2(\Omega)}) + Ch^2 (\|u\|_{H^1(\Omega)} + \|f\|_{H^1(\Omega)}) \|\tilde{w}_h\|_{H^1(\Omega)} \\
&+ Ch \|u\|_{H^2(\Omega_h)} (h \|w\|_{H^2(\Omega)} + h \|w\|_{H^2(\Omega_h)}) + Ch^2 (\|u\|_{H^1(\Omega_h)} + \|f\|_{H^1(\Omega_h)}) \|w_h\|_{H^1(\Omega_h)} \\
\le& Ch^2 (\|u\|_{H^2(\Omega)} + \|f\|_{H^1(\Omega)}) \|w\|_{H^2(\Omega)},
\end{aligned} \tag{3.51}$$

where we have used (3.46), and the facts that for $w \in H^1(\Omega)$, $v \in H^1(\Omega_h)$ there hold (cf. [13, eq. (5.16)], [8, Lemma 2 and Lemma 3] and [30, eq. (2.1) and (2.2)])

$$\|w\|_{L^2(\Omega\setminus\Omega_h)} \le Ch\|w\|_{H^1(\Omega)}, \quad \|v\|_{L^2(\Omega_h\setminus\Omega)} \le Ch\|v\|_{H^1(\Omega_h)}.$$

Furthermore, by using Lemma 3.6, (3.23), (3.24) and Lemma 3.8 we have

$$\begin{aligned}\langle \boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p - \tilde{w}_h, \partial_{\mathbf{n}}u - \widehat{\partial^h_{\mathbf{n}_h}u_h}\rangle_\Gamma =& \langle \boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p - \hat{Q}_h(\boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p), \partial_{\mathbf{n}}u - \widehat{\partial^h_{\mathbf{n}_h}u_h}\rangle_\Gamma \\ &+ \langle \hat{Q}_h(\boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p) - Q_h(\boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p\circ a_h)\circ a_h^{-1}, \partial_{\mathbf{n}}u - \widehat{\partial^h_{\mathbf{n}_h}u_h}\rangle_\Gamma \\ &+ \langle w_h\circ a_h^{-1} - \tilde{w}_h, \partial_{\mathbf{n}}u - \widehat{\partial^h_{\mathbf{n}_h}u_h}\rangle_\Gamma \\ \le& Ch^2\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p\|_{H^1(\Gamma)}(\|u\|_{W^{3,r}(\Omega)} + \|f\|_{H^1(\Omega)}).\end{aligned} \tag{3.52}$$

It remains to estimate $\langle u - u_h, \partial_{\mathbf{n}_h}w\rangle_{\Gamma_h}$. We conclude from (3.23) and (3.24) that

$$\begin{aligned}\langle u - u_h, \partial_{\mathbf{n}_h}w\rangle_{\Gamma_h} &\le \|g|_{\Gamma_h} - Q_h(g|_{\Gamma_h})\|_{L^2(\Gamma_h)}\|\partial_{\mathbf{n}_h}w\|_{L^2(\Gamma_h)} \\ &\le C\|g|_{\Gamma_h}\circ a_h^{-1} - Q_h(g|_{\Gamma_h})\circ a_h^{-1}\|_{L^2(\Gamma)}\|w\|_{H^2(\Omega)} \\ &\le C(\|g|_{\Gamma_h}\circ a_h^{-1} - \hat{Q}_h(g|_{\Gamma_h}\circ a_h^{-1})\|_{L^2(\Gamma)} + \|\hat{Q}_h(g|_{\Gamma_h}\circ a_h^{-1}) - Q_h(g|_{\Gamma_h})\circ a_h^{-1}\|_{L^2(\Gamma)})\|w\|_{H^2(\Omega)} \\ &\le Ch^2\|g\|_{H^2(\Gamma)}\|w\|_{H^2(\Omega)} \\ &\le Ch^2\|g\|_{H^3(\Omega)}\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p\|_{H^{\frac{3}{2}}(\Gamma)},\end{aligned} \tag{3.53}$$

where we used the fact that $u|_{\Gamma_h} = g|_{\Gamma_h}$ and $u_h|_{\Gamma_h} = Q_h(g|_{\Gamma_h})$ because we assumed in Assumption 2.1 that the Dirichlet boundary condition g is defined in $\mathbb{R}^n$. Thus, combining the above estimates we arrive at

$$\langle \boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p, \partial_{\mathbf{n}}u - \widehat{\partial^h_{\mathbf{n}_h}u_h}\rangle_\Gamma \le Ch^2\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}p\|_{H^{\frac{3}{2}}(\Gamma)}(\|u\|_{W^{3,r}(\Omega)} + \|f\|_{H^1(\Omega)} + \|g\|_{H^3(\Omega)}).$$

Similarly, we can prove

$$\langle \boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}u, \partial_{\mathbf{n}}p - \widehat{\partial^h_{\mathbf{n}_h}p_h}\rangle_\Gamma \le Ch^2\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}u\|_{H^{\frac{3}{2}}(\Gamma)}(\|u\|_{W^{3,r}(\Omega)} + \|f\|_{H^1(\Omega)} + \|g\|_{H^3(\Omega)} + \|p\|_{W^{3,r}(\Omega)})$$

and

$$\langle \boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}g, \partial_{\mathbf{n}}p - \widehat{\partial^h_{\mathbf{n}_h}p_h}\rangle_\Gamma \le Ch^2\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\partial_{\mathbf{n}}g\|_{H^{\frac{3}{2}}(\Gamma)}(\|u\|_{W^{3,r}(\Omega)} + \|f\|_{H^1(\Omega)} + \|g\|_{H^3(\Omega)} + \|p\|_{W^{3,r}(\Omega)}).$$

Moreover,

$$\begin{aligned}\langle \boldsymbol{\mathcal{V}}_{\mathbf{n}}(\partial_{\mathbf{n}}u - \widehat{\partial^h_{\mathbf{n}_h}u_h}), \partial_{\mathbf{n}}p - \widehat{\partial^h_{\mathbf{n}_h}p_h}\rangle_\Gamma &\le \|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)}\|\partial_{\mathbf{n}}p - \widehat{\partial^h_{\mathbf{n}_h}p_h}\|_{L^2(\Gamma)}\|\partial_{\mathbf{n}}u - \widehat{\partial^h_{\mathbf{n}_h}u_h}\|_{L^2(\Gamma)} \\ &\le Ch^2\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{H^{\frac{3}{2}}(\Gamma)}(\|u\|_{W^{3,r}(\Omega)} + \|f\|_{H^1(\Omega)} + \|g\|_{H^3(\Omega)} + \|p\|_{W^{3,r}(\Omega)})^2.\end{aligned}$$

Combining the above results we have $|J_1| \le Ch^2$, this together with $|J_2| \le Ch^2$ gives the result. ◻

In the following we discuss the possible extension of the results in Theorem 3.10 to the convex polygonal domains.

Remark 3.11. *First we recall the regularity results of the solution to the elliptic equations (2.2) with Dirichlet boundary conditions. Let Ω be a convex polygonal domain with Lipschitz boundary Γ and f, g be smooth enough in $\mathbb{R}^2$. We denote by $\frac{\pi}{3} \le \omega_1 < \pi$ the largest interior angle of Γ, and by*

$$s_\Omega = \frac{2}{2 - \min\{2, \frac{\pi}{\omega_1}\}} > 2, \quad r_\Omega = 1 + \pi/\omega_1 \in (2, 4]$$

the exponents giving the maximal regularity to the solution of (2.2) in $W^{2,s}(\Omega)$ for $s < s_\Omega$ ([23, Theorem 4.4.3.7]) and $H^r(\Omega)$ for $r < r_\Omega$ ([23, Theorem 5.1.1.4]) if f and g are smooth enough. In the case $n = 3$, s_Ω and r_Ω have more complicated expressions depending on interior angles of both edges and corners of the polyhedron; see [18, Corollary 3.9 and Section 4.c]. The above regularity also applies to the adjoint state equation (2.5) if $j'(u)$ is sufficiently smooth.

In particular, the formulas (3.13) and (3.14) are well-defined. In fact, taking the state u as an example, if Ω is a convex polygonal domain and $g = 0$ we have $u \in W^{2,s}(\Omega) \cap H^1_0(\Omega)$ and thus $\partial_{\mathbf{n}}u \in W^{1-1/s,s}(\Gamma)$ (We refer to [12, Theorem 3.4] where $u \in H^1_0(\Omega)$ plays a crucial role in deriving $\partial_{\mathbf{n}}u \in W^{1-1/s,s}(\Gamma)$). If $g \neq 0$ we may need some compatibility condition for g to derive $\partial_{\mathbf{n}}u \in W^{1-1/s,s}(\Gamma)$.

We remark that the proof for the improved convergence rate of the discrete shape gradients of boundary type by using the corrected outward normal derivatives relies on the L^2- and H^1-norm error estimates (3.6), the

$W^{1,\infty}$-norm error estimate (3.8), the first order convergence of the outward norm derivative approximations in Lemma 3.8, the regularity $\mathcal{V}_{\mathbf{n}}\partial_{\mathbf{n}}p, \mathcal{V}_{\mathbf{n}}\partial_{\mathbf{n}}u, \mathcal{V}_{\mathbf{n}}\partial_{\mathbf{n}}g \in H^{\frac{3}{2}}(\Gamma)$ which in turn ensures the $H^2(\Omega)$ regularity for the solution w to problem (3.43) and the error estimates (3.46).

Specifically, (3.6) can be achieved for a convex polygonal domain, while the $W^{2,\infty}$ regularity for u and p imposes restriction to the maximal interior angle ω_1, i.e., $\omega_1 \in [\frac{\pi}{3}, \frac{\pi}{2})$. Further, if $u, p \in H^3(\Omega) \cap H_0^1(\Omega)$ and $g = 0$ we can expect $\mathcal{V}_{\mathbf{n}}\partial_{\mathbf{n}}p, \mathcal{V}_{\mathbf{n}}\partial_{\mathbf{n}}u \in H^{\frac{3}{2}-\varepsilon}(\Gamma)$, because $\mathcal{V}_{\mathbf{n}}\partial_{\mathbf{n}}p, \mathcal{V}_{\mathbf{n}}\partial_{\mathbf{n}}u$ are piecewise $H^{\frac{3}{2}}$ on Γ and $\partial_{\mathbf{n}}p$ and $\partial_{\mathbf{n}}u$ vanish at the corners. For the approximation of the outward normal derivative in general polygonal domain we can only expect ([12])

$$\|\partial_{\mathbf{n}}u - \partial_{\mathbf{n}}^h u_h\|_{L^2(\Gamma)} \leq Ch^{1-\frac{1}{s}}\|u\|_{W^{2,s}(\Omega)}.$$

However, the above error estimate can be improved to be $O(h^{1-\varepsilon})$ for any $\varepsilon > 0$ if the maximum angle of Ω is smaller than $\frac{2\pi}{3}$ (cf. [4, Figure 1 and Theorem 4.1]). Furthermore, the order can be improved to be $O(h^{1.5-\varepsilon})$ (cf. [4, Figure 1 and Theorem 4.1]) if the maximum angle of Ω is smaller than $\frac{\pi}{2}$ and the mesh satisfies the super-convergence property, i.e., is of $O(h^{2\sigma})$ (cf. [15]).

In conclusion, it seems that we can not prove second order convergence for the modified shape gradient in a general polygonal domain. However, in the case that f, g are smooth enough and $\omega_1 \in [\frac{\pi}{3}, \frac{\pi}{2})$ we can expect almost second order convergence rate. The first example (Example 1) in Section 4 shows this optimal second order convergence rate, while the third example (Example 3) shows a better result than that we expect.

3.2. Neumann boundary value problem. In this subsection we consider the Neumann boundary value problem. For the state equation (2.2) with Neumann boundary condition, the weak formulation is to find $u \in H^1(\Omega)$ such that

$$(\nabla u, \nabla v) + (u, v) = (f, v) + \langle g, v\rangle_\Gamma \quad \forall v \in H^1(\Omega). \tag{3.54}$$

The finite element approximation of (3.54) reads: find $u_h \in V_h \subset H^1(\Omega_h)$ such that

$$(\nabla u_h, \nabla v_h)_h + (u_h, v_h)_h = (f, v_h)_h + \langle g, v_h\rangle_{\Gamma_h} \quad \forall v_h \in V_h. \tag{3.55}$$

Similarly, the variational weak formulation of (2.5) is to find $p \in H^1(\Omega)$ such that

$$(\nabla p, \nabla v) + (p, v) = (j'(u), v) \quad \forall v \in H^1(\Omega), \tag{3.56}$$

while its finite element approximation reads: find $p_h \in V_h \subset H^1(\Omega_h)$ such that

$$(\nabla p_h, \nabla v_h)_h + (p_h, v_h)_h = (j'(u_h), v_h)_h \quad \forall v_h \in V_h. \tag{3.57}$$

To use known results in the literature we use a slightly different lifting operator (cf. [19, 30]) from that used in Section 3.1. As an embedded, compact hypersurface in $\mathbb{R}^n$, Γ is orientable with a unit normal field $\mathbf{n}$ pointing to the outside of the domain Ω and hence can be represented by the zero level set of the signed distance function d such that (cf. [17])

$$|d(x)| = \mathrm{dist}(x, \Gamma) \quad \text{and} \quad \mathbf{n}(x) = \frac{\nabla d(x)}{\|\nabla d(x)\|} \quad \text{for } x \in \Gamma.$$

Furthermore, one can find a neighborhood $U \subset \mathbb{R}^n$ of Γ, such that d is also of class C^3 on U and the projection $a : \Gamma_h \to \Gamma$ is well defined by

$$a(x) := x - d(x)\nabla d(x), \quad x \in \Gamma_h$$

such that $\nabla d(x) = \mathbf{n}(a(x))$, and a can be extended as a mapping from U to Γ. Then one can show that $\|d\|_{L^\infty(\Gamma_h)} \leq Ch^2$ and $\|1 - \delta_h\|_{L^\infty(\Gamma_h)} \leq Ch^2$ (cf. [19, Lemma 4.1]) where δ_h denotes the quotient between the smooth and discrete surface measures ds and ds_h, i.e., $\delta_h ds_h = ds$. The main difference between the projection mapping $a(x)$ defined in this subsection with the one $a_h(x)$ defined in (3.15) lies in the normal directions. Specifically, in the definition (3.15) the projection $a_h(x)$ is along the normal direction of Γ_h, while the projection $a(x)$ used in this subsection is along the normal direction of Γ.

For any function v_h defined on Γ_h we can define the lifting v_h^l on Γ as $v_h^l(a(x)) = v_h(x)$. Similarly, for any function v defined on Γ we can define the inverse lifting v^{-l} on Γ_h as $v^{-l}(x) = v(a(x)) = v \circ a(x)$. Then there holds $(v^{-l})^l = v$. On Γ_h we define for $v_h \in V_h(\Gamma_h)$ the tangential operator $\nabla_{\Gamma_h} v_h := \nabla v_h - (\nabla v_h \cdot \mathbf{n}_h)\mathbf{n}_h = P_h \nabla v_h$, where $(P_h)_{i,k} = \delta_{ik} - \mathbf{n}_{h,i}\mathbf{n}_{h,k}$, $i, k = 1, 2$. From the definition of v_h^l we have $\nabla v_h = (P - dH)\nabla(v_h^l) \circ a$ with $P_{i,k} = \delta_{i,k} - \mathbf{n}_i\mathbf{n}_k$ and $H_{i,k} = \partial_{x_i x_k} d = \partial_{x_k}\mathbf{n}_i = \partial_{x_i}\mathbf{n}_k$. Using the property $PH = HP = H$ we obtain (cf. [19, Lemma 4.2])

$$\nabla_{\Gamma_h} v_h(x) = P_h(x)(\mathbb{I} - d(x)H(x))P(x)\nabla v_h^l(a(x)) = P_h(x)(\mathbb{I} - d(x)H(x))\nabla_\Gamma v_h^l(a(x)) \quad \text{on } \Gamma_h. \tag{3.58}$$

Then one has the following stabilities for the lifting operator (cf. [19, Lemma 4.2]):

$$\begin{aligned} \frac{1}{C}\|v\|_{L^2(\Gamma_h)} \le \|v^l\|_{L^2(\Gamma)} \le C\|v\|_{L^2(\Gamma_h)}, \\ \frac{1}{C}\|\nabla_{\Gamma_h} v\|_{L^2(\Gamma_h)} \le \|\nabla_\Gamma v^l\|_{L^2(\Gamma)} \le C\|\nabla_{\Gamma_h} v\|_{L^2(\Gamma_h)}. \end{aligned} \tag{3.59}$$

Now we are ready to define the approximate shape gradient to (2.11):

$$\mathrm{d}_h J^N(\Gamma_h, u_h, p_h; \boldsymbol{\mathcal{V}}) = \int_{\Gamma_h} \boldsymbol{\mathcal{V}}_\mathbf{n} \circ a\Big(j(u_h) - \nabla_{\Gamma_h} u_h \cdot \nabla_{\Gamma_h} p_h - u_h p_h + (f + \partial_\mathbf{n} g \circ a + K \circ a g) p_h\Big) ds_h, \tag{3.60}$$

where ∇_{Γ_h} denotes the tangential gradient on Γ_h.

Remark 3.12. *The definition (3.60) involves the mapping a between Γ_h and Γ, which is not trivial to compute explicitly. In the special case of implicitly defined domain (cf. [19, Sections 7 and 8]), the boundary Γ is the zero level set of the signed distance function d and thus the mapping a can be explicitly computed. In the general case, we usually compute the integral (3.60) by using quadrature formula, thus we only need to evaluate $a(x)$ at finite many points which is obviously possible when the representation of Γ is available by recalling that $\nabla d(x) = \mathbf{n}(a(x))$.*

It was numerically observed in [29] that the approximate shape gradient in the boundary formulation of the Eulerian derivative for the Neumann boundary value problem has the same convergence rate and accuracy as that for the volume formulation on convex polygon or smooth domain having C^2 boundary. For such domains, however, the theoretical analysis therein shows that the discrete boundary formulation has lower convergence rate than the volumetric formulation when the data is smooth. In this subsection, we prove that the boundary shape gradient has nearly the same convergence rate as in the volume case for the Neumann boundary value problem, when the solution is sufficiently regular.

Converting (3.60) to Γ we have (cf. [19, Lemma 4.7])

$$\begin{aligned} &\tilde{\mathrm{d}}_h J^N(\Gamma, u_h, p_h; \boldsymbol{\mathcal{V}}) \\ &= \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}\Big(j(u_h^l) - P_h(\mathbb{I} - dH)\nabla_\Gamma u_h^l \cdot P_h(\mathbb{I} - dH)\nabla_\Gamma p_h^l - u_h^l p_h^l + (f + \partial_\mathbf{n} g + Kg)p_h^l\Big)\frac{1}{\delta_h} ds \\ &= \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}\Big(j(u_h^l) - \nabla_\Gamma u_h^l \cdot \nabla_\Gamma p_h^l - u_h^l p_h^l + (f + \partial_\mathbf{n} g + Kg)p_h^l\Big) ds \\ &\quad + \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}(\mathbb{I} - B_h)\nabla_\Gamma u_h^l \cdot \nabla_\Gamma p_h^l ds + \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}(\frac{1}{\delta_h} - 1)\Big(j(u_h^l) - u_h^l p_h^l + (f + \partial_\mathbf{n} g + Kg)p_h^l\Big) ds, \end{aligned}$$

where (cf. [19, P. 317, proof of Lemma 4.7])

$$B_h = \frac{1}{\delta_h}(\mathbb{I} - dH)PP_hP(\mathbb{I} - dH) = \frac{1}{\delta_h}P(\mathbb{I} - dH)P_h(\mathbb{I} - dH)P$$

since P is a projection.

Theorem 3.13. *Let u and p be the continuous solutions to the state equation (3.54) and adjoint equation (3.56) with Neumann boundary conditions, while u_h and p_h denote the discrete solutions to (3.55) and (3.57), respectively. Assume that Assumption 2.1 holds and $u, p \in W^{3,r}(\Omega)$ for some $r > n$, we have*

$$\begin{aligned} |\mathrm{d}J^N(\Gamma, u, p; \boldsymbol{\mathcal{V}}) - \tilde{\mathrm{d}}_h J^N(\Gamma, u_h, p_h; \boldsymbol{\mathcal{V}})| \le & Ch^2|\log h|\|\boldsymbol{\mathcal{V}}_\mathbf{n}\|_{W^{1,\infty}(\Gamma)}(\|u\|_{W^{2,\infty}(\Omega)} \\ & + \|p\|_{W^{2,\infty}(\Omega)})(\|u\|_{W^{2,\infty}(\Omega)} + \|f\|_{H^1(\Omega)} + \|g\|_{H^2(\Omega)}). \end{aligned} \tag{3.61}$$

Proof. From the definition we have

$$\begin{aligned} &\mathrm{d}J^N(\Gamma, u, p; \boldsymbol{\mathcal{V}}) - \tilde{\mathrm{d}}_h J^N(\Gamma, u_h, p_h; \boldsymbol{\mathcal{V}}) \\ &= \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}\big((j(u) - j(u_h^l)) - (up - u_h^l p_h^l) + (f + \partial_\mathbf{n} g + Kg)(p - p_h^l)\big) ds \\ &\quad - \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}(\nabla_\Gamma u \cdot \nabla_\Gamma p - \nabla_\Gamma u_h^l \cdot \nabla_\Gamma p_h^l) ds - \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}(\mathbb{I} - B_h)\nabla_\Gamma u_h^l \cdot \nabla_\Gamma p_h^l ds \\ &\quad - \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}\Big(\frac{1}{\delta_h} - 1\Big)\Big(j(u_h^l) - u_h^l p_h^l + (f + \partial_\mathbf{n} g + Kg)p_h^l\Big) ds. \end{aligned} \tag{3.62}$$

Now it remains to estimate the right-hand side. First, it follows from Lemma 4.7 in [19] that

$$\begin{aligned} \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}(\mathbb{I} - B_h)\nabla_\Gamma u_h^l \cdot \nabla_\Gamma p_h^l ds &= \int_\Gamma \boldsymbol{\mathcal{V}}_\mathbf{n}(P - B_h)\nabla_\Gamma u_h^l \cdot \nabla_\Gamma p_h^l ds \\ &\le Ch^2\|\boldsymbol{\mathcal{V}}_\mathbf{n}\|_{L^\infty(\Gamma)}\|u\|_{W^{1,\infty}(\Omega)}\|p\|_{W^{1,\infty}(\Omega)}, \end{aligned} \tag{3.63}$$

where we used the fact that $|P - B_h| \le Ch^2$ on Γ. Second, using $\|1-\delta_h\|_{L^\infty(\Gamma_h)} \le Ch^2$ and the stability results (3.59) one can derive

$$\int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} \Big(\frac{1}{\delta_h} - 1\Big)\Big(j(u_h^l) - u_h^l p_h^l + (f + \partial_{\mathbf{n}} g + Kg)p_h^l\Big) ds \le Ch^2 \|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)} \Big(\|u\|_{H^1(\Omega)} + (\|u\|_{H^1(\Omega)} + \|f\|_{H^1(\Omega)} + \|g\|_{H^2(\Omega)})\|p\|_{H^1(\Omega)}\Big). \tag{3.64}$$

Note that for our case of C^3 domain Ω and sufficiently smooth data f and g, we have the $W^{2,\infty}(\Omega)$ regularity for the solutions u and p to the state and adjoint equations. Denote by $\tilde{u}, \tilde{p}$ their continuous extensions to $\mathbb{R}^n$ satisfying (3.1), we thus have $\tilde{u}, \tilde{p} \in W^{2,\infty}(\Omega_h)$. In the following we will derive the estimates for $\|u - \tilde{u}^l\|_{L^2(\Gamma)}$ and $\|p - \tilde{p}^l\|_{L^2(\Gamma)}$.

It follows from (3.59) and [30, eq. (2.1) with $p = 2$] that

$$\|u - \tilde{u}^l\|_{L^2(\Gamma)} \le C\|u^{-l} - \tilde{u}\|_{L^2(\Gamma_h)} \le Ch\|\nabla \tilde{u}\|_{L^2(U)} \le Ch(h\|\nabla \tilde{u}\|_{L^2(\Gamma)} + h^2\|\nabla^2 \tilde{u}\|_{L^2(U)}), \tag{3.65}$$

which together with (3.1), (3.59) and the L^∞-norm error estimate [30, Theorem 3.1] gives

$$\begin{aligned} \|u - u_h^l\|_{L^2(\Gamma)} &\le \|u - \tilde{u}^l\|_{L^2(\Gamma)} + \|\tilde{u}^l - u_h^l\|_{L^2(\Gamma)} \\ &\le Ch^2\|u\|_{H^2(\Omega)} + C\|\tilde{u} - u_h\|_{L^2(\Gamma_h)} \\ &\le Ch^2\|u\|_{H^2(\Omega)} + C\|\tilde{u} - u_h\|_{L^\infty(\Omega_h)} \\ &\le Ch^2\|u\|_{H^2(\Omega)} + Ch^2|\log h|\|u\|_{W^{2,\infty}(\Omega)} \\ &\le Ch^2|\log h|\|u\|_{W^{2,\infty}(\Omega)}. \end{aligned} \tag{3.66}$$

As for the adjoint state variable p, we can proceed similarly as above

$$\begin{aligned} \|p - p_h^l\|_{L^2(\Gamma)} &\le \|p - \tilde{p}^l\|_{L^2(\Gamma)} + \|\tilde{p}^l - p_h^l\|_{L^2(\Gamma)} \\ &\le Ch^2\|p\|_{H^2(\Omega)} + C\|\tilde{p} - p_h\|_{L^2(\Gamma_h)} \\ &\le Ch^2\|p\|_{H^2(\Omega)} + C\|\tilde{p} - p_h(u)\|_{L^2(\Gamma_h)} + C\|p_h(u) - p_h\|_{L^2(\Gamma_h)} \\ &\le Ch^2\|p\|_{H^2(\Omega)} + C\|\tilde{p} - p_h(u)\|_{L^\infty(\Omega_h)} + C\|j'\|_{C^{0,1}(I)}\|\tilde{u} - u_h\|_{L^2(\Omega_h)} \\ &\le Ch^2\|p\|_{H^2(\Omega)} + C\|\tilde{p} - p_h(u)\|_{L^\infty(\Omega_h)} + C\|\tilde{u} - u_h\|_{L^\infty(\Omega_h)} \\ &\le Ch^2|\log h|(\|u\|_{W^{2,\infty}(\Omega)} + \|p\|_{W^{2,\infty}(\Omega)}), \end{aligned} \tag{3.67}$$

where $p_h(u) \in V_h$ is defined similarly as in Remark 3.3, and I is also defined as in Remark 3.3.

Then we have

$$\begin{aligned} \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} |j(u) - j(u_h^l)| ds &\le C\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)}\|j\|_{C^{0,1}(I)}\|u - u_h^l\|_{L^1(\Gamma)} \\ &\le C\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)}\|j\|_{C^{0,1}(I)}\|u - u_h^l\|_{L^2(\Gamma)} \\ &\le Ch^2|\log h|\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)}\|j\|_{C^{0,1}(I)}\|u\|_{W^{2,\infty}(\Omega)}. \end{aligned}$$

Moreover, it holds

$$\begin{aligned} &\int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}}(up - u_h^l p_h^l) ds \\ =& \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}}(p(u - u_h^l) + u(p - p_h^l) - (u - u_h^l)(p - p_h^l)) ds \\ \le& \|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)}(\|p\|_{L^2(\Gamma)}\|u - u_h^l\|_{L^2(\Gamma)} + \|u\|_{L^2(\Gamma)}\|p - p_h^l\|_{L^2(\Gamma)} + \|u - u_h^l\|_{L^2(\Gamma)}\|p - p_h^l\|_{L^2(\Gamma)}) \\ \le& Ch^2|\log h|\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)}\|u\|_{W^{2,\infty}(\Omega)}(\|u\|_{W^{2,\infty}(\Omega)} + \|p\|_{W^{2,\infty}(\Omega)}) \end{aligned}$$

and

$$\begin{aligned} \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}}(f + Kg)(p - p_h^l) ds &\le \|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)}\|f + Kg\|_{L^2(\Gamma)}\|p - p_h^l\|_{L^2(\Gamma)} \\ &\le Ch^2|\log h|\|\boldsymbol{\mathcal{V}}_{\mathbf{n}}\|_{L^\infty(\Gamma)}(\|u\|_{W^{2,\infty}(\Omega)} + \|p\|_{W^{2,\infty}(\Omega)})(\|f\|_{H^1(\Omega)} + \|g\|_{H^2(\Omega)}). \end{aligned} \tag{3.68}$$

By the tangential Green's formula [19, Theorem 2.14]

$$\int_\Gamma (w \operatorname{div}_\Gamma \mathbf{v} + \nabla_\Gamma w \cdot \mathbf{v}) ds = \int_\Gamma Kw\mathbf{v} \cdot \mathbf{n} ds \tag{3.69}$$

for a function $w \in H^1(\Gamma)$ and vector $\mathbf{v} \in H^1(\Gamma)^n$, we have

$$\begin{aligned}
&\int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} (\nabla_\Gamma u \cdot \nabla_\Gamma p - \nabla_\Gamma u_h^l \cdot \nabla_\Gamma p_h^l) ds \\
&= \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} \Big(\nabla_\Gamma u \cdot \nabla_\Gamma (p - p_h^l) + \nabla_\Gamma p \cdot \nabla_\Gamma (u - u_h^l) - \nabla_\Gamma (u - u_h^l) \cdot \nabla_\Gamma (p - p_h^l) \Big) ds \\
&= - \int_\Gamma \operatorname{div}_\Gamma (\boldsymbol{\mathcal{V}}_{\mathbf{n}} \nabla_\Gamma u)(p - p_h^l) ds - \int_\Gamma \operatorname{div}_\Gamma (\boldsymbol{\mathcal{V}}_{\mathbf{n}} \nabla_\Gamma p)(u - u_h^l) ds \\
&\quad - \int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} \nabla_\Gamma (u - u_h^l) \cdot \nabla_\Gamma (p - p_h^l) ds.
\end{aligned} \tag{3.70}$$

Then, we estimate the three terms on the right-hand side. First, using (3.67) we have

$$\begin{aligned}
\int_\Gamma \operatorname{div}_\Gamma (\boldsymbol{\mathcal{V}}_{\mathbf{n}} \nabla_\Gamma u)(p - p_h^l) ds &\le \| \operatorname{div}_\Gamma (\boldsymbol{\mathcal{V}}_{\mathbf{n}} \nabla_\Gamma u) \|_{L^2(\Gamma)} \| p - p_h^l \|_{L^2(\Gamma)} \\
&\le Ch^2 |\log h| \| \boldsymbol{\mathcal{V}}_{\mathbf{n}} \|_{W^{1,\infty}(\Gamma)} \| u \|_{H^{5/2}(\Omega)} (\| u \|_{W^{2,\infty}(\Omega)} + \| p \|_{W^{2,\infty}(\Omega)}).
\end{aligned} \tag{3.71}$$

Similarly, it follows from (3.66) that

$$\begin{aligned}
\int_\Gamma \operatorname{div}_\Gamma (\boldsymbol{\mathcal{V}}_{\mathbf{n}} \nabla_\Gamma p)(u - u_h^l) ds &\le \| \operatorname{div}_\Gamma (\boldsymbol{\mathcal{V}}_{\mathbf{n}} \nabla_\Gamma p) \|_{L^2(\Gamma)} \| u - u_h^l \|_{L^2(\Gamma)} \\
&\le Ch^2 |\log h| \| \boldsymbol{\mathcal{V}}_{\mathbf{n}} \|_{W^{1,\infty}(\Gamma)} \| p \|_{H^{5/2}(\Omega)} \| u \|_{W^{2,\infty}(\Omega)}.
\end{aligned} \tag{3.72}$$

Furthermore, it follows from the triangle inequality, the definition of $\nabla_{\Gamma_h} v$, the stability results (3.1) and (3.59), the estimate (3.65) and an $W^{1,\infty}$ error estimate (cf. [30, Theorem 3.1]) that

$$\begin{aligned}
\| \nabla_\Gamma (u - u_h^l) \|_{L^2(\Gamma)} &\le \| \nabla_\Gamma (u - \tilde{u}^l) \|_{L^2(\Gamma)} + \| \nabla_\Gamma (\tilde{u}^l - u_h^l) \|_{L^2(\Gamma)} \\
&\le C \| \nabla_{\Gamma_h} (u^{-l} - \tilde{u}) \|_{L^2(\Gamma_h)} + C \| \nabla_{\Gamma_h} (\tilde{u} - u_h) \|_{L^2(\Gamma_h)} \\
&\le C \| \nabla (u^{-l} - \tilde{u}) \|_{L^2(\Gamma_h)} + C \| \tilde{u} - u_h \|_{W^{1,\infty}(\Omega_h)} \\
&\le Ch \| \nabla^2 \tilde{u} \|_{L^2(U)} + Ch \| u \|_{W^{2,\infty}(\Omega)} \\
&\le Ch \| u \|_{W^{2,\infty}(\Omega)}.
\end{aligned} \tag{3.73}$$

A similar argument as above and proceeding as in the estimate of $\| p - p_h^l \|_{L^2(\Gamma)}$ yield

$$\| \nabla_\Gamma (p - p_h^l) \|_{L^2(\Gamma)} \le Ch (\| u \|_{W^{2,\infty}(\Omega)} + \| p \|_{W^{2,\infty}(\Omega)}). \tag{3.74}$$

Finally, we have

$$\begin{aligned}
\int_\Gamma \boldsymbol{\mathcal{V}}_{\mathbf{n}} \nabla_\Gamma (u - u_h^l) \cdot \nabla_\Gamma (p - p_h^l) ds &\le C \| \boldsymbol{\mathcal{V}}_{\mathbf{n}} \|_{L^\infty(\Gamma)} \| \nabla_\Gamma (u - u_h^l) \|_{L^2(\Gamma)} \| \nabla_\Gamma (p - p_h^l) \|_{L^2(\Gamma)} \\
&\le Ch^2 \| \boldsymbol{\mathcal{V}}_{\mathbf{n}} \|_{L^\infty(\Gamma)} \| u \|_{W^{2,\infty}(\Omega)} (\| u \|_{W^{2,\infty}(\Omega)} + \| p \|_{W^{2,\infty}(\Omega)}).
\end{aligned} \tag{3.75}$$

Combining the above estimates we finish the proof. □

The above error estimates indicate that when the solutions are sufficiently smooth, we can expect almost second order convergence for the approximate boundary formulation of the shape gradient for Neumann boundary value problems. This partially confirms the numerical observations in [29], whereas the theoretical analysis therein fails to prove this convergence rate.

4. Numerical results. In this section we present some numerical results to verify the convergence rate of finite element approximations to shape gradients with boundary corrections.

We numerically verify the theoretical results in Theorem 3.10. The shape gradient for shape functional is a linear continuous operator on $H^{3/2}(\mathbb{R}^n; \mathbb{R}^n)$ and belongs to its dual space in either the volume or the boundary type Eulerian derivative. It is challenging to compute numerically the continuous infinite-dimensional operator norm for the approximate shape gradients. This norm can be approximately replaced by a tractable one on a finite-dimensional subspace. More precisely, given a positive integer γ as in [29], we consider an approximate operator norm on a finite-dimensional space consisting of vector fields in $\mathcal{P}_\gamma(\mathbb{R}^n; \mathbb{R}^n) (\subset H^{3/2}(\mathbb{R}^n; \mathbb{R}^n))$, whose components are multivariate polynomials of degree up to γ. Based on the equivalence of norms over finite-dimensional spaces, we replace the $H^{3/2}$-norm with a more tractable H^1-norm. Finally, we compute the approximate dual norms

$$\mathcal{E} := \left(\max_{0 \neq \boldsymbol{\mathcal{V}} \in \mathcal{P}_\gamma(\mathbb{R}^n; \mathbb{R}^n)} \frac{|\mathrm{d}J^D(\Gamma, u, p; \boldsymbol{\mathcal{V}}) - \tilde{\mathrm{d}}_h J^D(\Gamma, u_h, p_h; \boldsymbol{\mathcal{V}})|^2}{\| \boldsymbol{\mathcal{V}} \|_{H^1(\Omega)}^2} \right)^{1/2}. \tag{4.1}$$

We take a global basis $\{\boldsymbol{\mathcal{V}}_i\}_{i=1}^q$ of vector fields in $\mathcal{P}_\gamma(\mathbb{R}^n;\mathbb{R}^n)$, where $q = nC_{\gamma+n}^n$ with $C_{\gamma+n}^n$ denoting the combination coefficient. More precisely, we choose

$$\{\boldsymbol{\mathcal{V}}_i\}_{i=1}^q = \left\{[\Pi_{i=1}^n x_i^{\beta_i}, 0, \cdots, 0], \cdots, [0, \cdots, 0, \Pi_{i=1}^n x_i^{\beta_i}]\right\}_{\sum_{i=1}^n \beta_i \le \gamma},$$

where β_i $(i = 1, \cdots, n)$ are non-negative integers. We denote the Gramian matrix associated with the $H^1(\Omega)$ inner product by $\mathbb{K} = [(\boldsymbol{\mathcal{V}}_i, \boldsymbol{\mathcal{V}}_k)_{H^1(\Omega)}]_{i,k=1}^q \in \mathbb{R}^{q\times q}$. The errors (4.1) can be obtained by

$$\mathcal{E} := \left(w^T \mathbb{K}^{-1} w\right)^{1/2}, \tag{4.2}$$

where

$$w := [\mathrm{d}J^D(\Gamma, u, p; \boldsymbol{\mathcal{V}}_i) - \tilde{\mathrm{d}}_h J^D(\Gamma, u_h, p_h; \boldsymbol{\mathcal{V}}_i)]_{i=1}^q.$$

In the following examples we set $u_{\mathrm{d}} = 0$ and use the cost functional $J(\Omega) = \frac{1}{2}\int_\Omega u^2 dx$, so that $j(u) := \frac{1}{2}u^2$. We construct **Example 1** with

$$u(x_1, x_2) = \cos\left(\frac{\pi}{2}x_1\right)\cos\left(\frac{\pi}{2}x_2\right), \quad f = \left(\frac{1}{2}\pi^2 + 1\right)\cos\left(\frac{\pi}{2}x_1\right)\cos\left(\frac{\pi}{2}x_2\right)$$

on $\Omega = (-1, 1)^2$ and set g accordingly. The adjoint state has exact solution

$$p(x_1, x_2) = \frac{1}{2\pi^2 + 4}\cos\left(\frac{\pi}{2}x_1\right)\cos\left(\frac{\pi}{2}x_2\right).$$

In the following, we use a numerical solution on a very fine mesh as reference for computing numerical errors. In **Example 2**, we set Ω to be a disk of radius $\sqrt{\pi}$ centered at the origin. We choose

$$u(x_1, x_2) = \cos(x_1)\cos(x_2), \quad f = 3\cos(x_1)\cos(x_2)$$

and set inhomogeneous Dirichlet boundary condition $g = \cos(x_1)\cos(x_2)$. In this example with a curved computational domain, the vector field $\boldsymbol{\mathcal{V}}_{\mathbf{n}}$ was not composed with a_h when using the formula (3.10), however, we still observe second order convergence. In **Example 3**, we choose Ω to be an irregular convex polygon intersected by four lines: $x_1 = 0$, $x_2 = 0$, $x_2 = -\sqrt{3}x_1 + \sqrt{3}$, and $x_2 = (\sqrt{3} - 2)x_1 + 1$, such that the maximum interior angle is larger than $90°$. We set

$$f = \mathrm{e}^{-x_1^2 x_2}\cos(x_1)\sin(x_2)$$

and $g = 0$. Both solutions to the state and adjoint equation are unknown. In **Example 4**, we choose a domain that does not guarantee H^2-regularity of the state problem. We set a L-shaped domain with a reentrant corner $\Omega = (-1, 1)^2 \setminus \{[0, 1) \times (-1, 0]\}$. The source function is, in polar coordinates, $f(x) = r^{2/3}\sin(2\theta/3)$ with $r = \sqrt{x_1^2 + x_2^2}$ and θ being the polar angle. Choose $g = 0$. In Fig. 4.1, we show the finite element approximations of the state equations for domains associated with the three examples.

For **Examples 1-3**, we see from Fig. 4.2 that the errors committed by shape gradients with boundary correction converge quadratically, while the errors of those without boundary correction converge linearly. When the domain is nonconvex, so that the solution is not sufficiently regular (not in $H^2(\Omega)$) as for **Example 4**, Fig. 4.2 (the third subplot) shows that the shape gradient with boundary correction converges faster than the classical one, but with a rate less than 2, this is in agreement with that of the volume one (cf. [29]). The parameter γ has no obvious effect on convergence as shown in Fig. 4.3.

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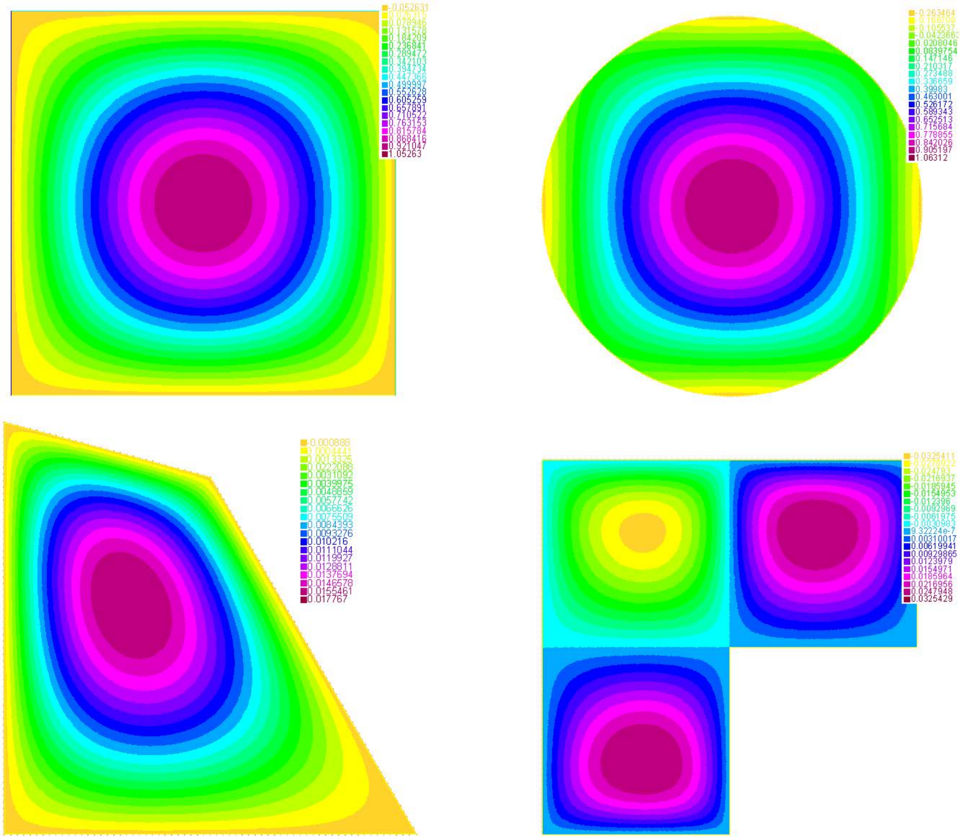

FIG. 4.1. *Four computational domains and the according finite element solutions for Example 1, Example 2, Example 3, and Example 4, respectively.*

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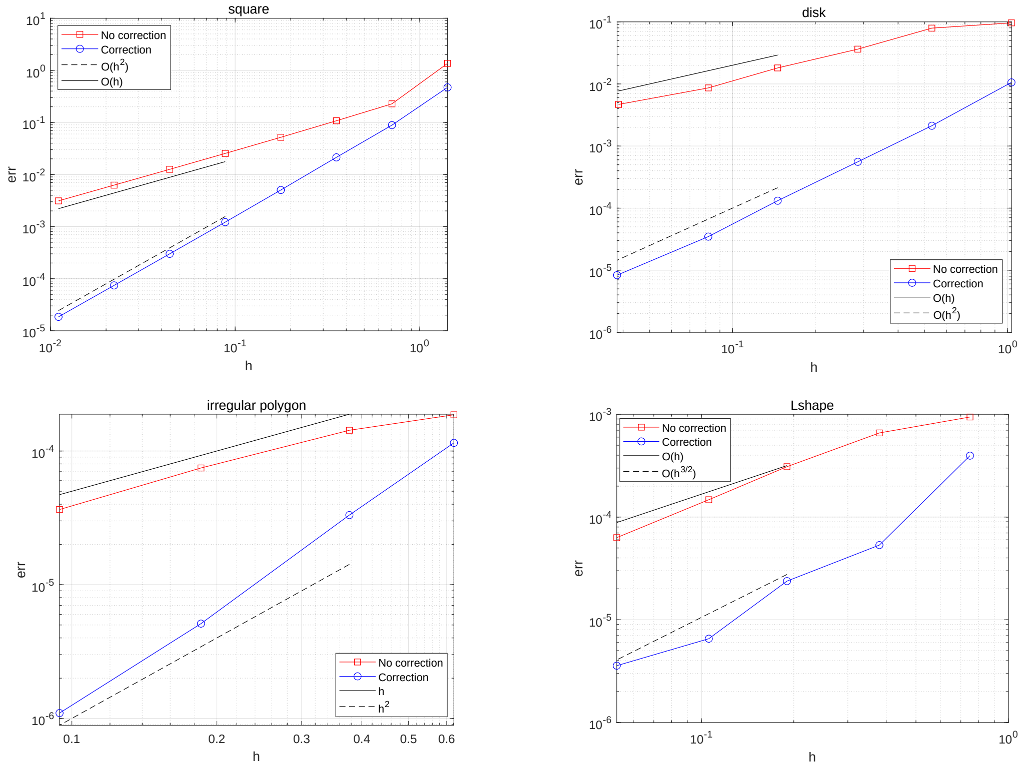

FIG. 4.2. *The convergence history of approximate shape gradients with* $\gamma = 3$.

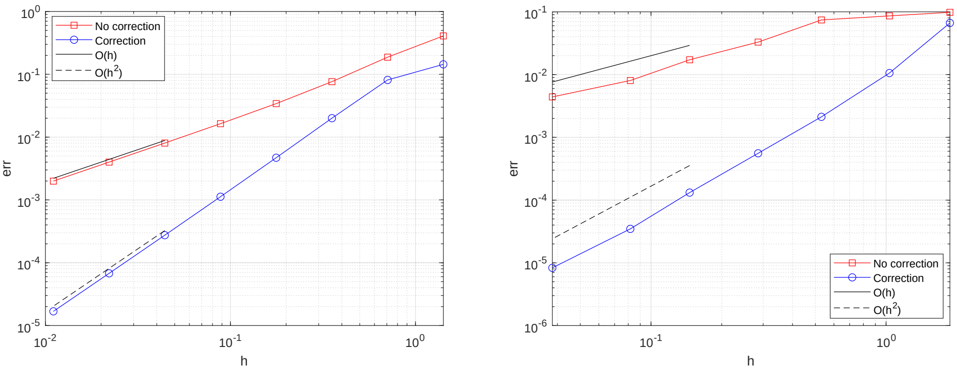

FIG. 4.3. *The convergence history of approximate shape gradients with* $\gamma = 2$*: square (left) and disk (right).*

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