UNFITTED FINITE ELEMENT METHODS FOR SHAPE OPTIMIZATION AND LIQUID CRYSTALS

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Table of Contents

List of Tables

List of Figures

Abstract

We present an approach to shape optimization problems that uses an unfitted finite element method (FEM). The domain geometry is represented, and optimized, using a (discrete) level set function and we consider objective functionals that are defined over bulk domains. For a discrete objective functional, defined in the unfitted FEM framework, we show that the *exact* discrete shape derivative essentially matches the shape derivative at the continuous level. In other words, our approach has the benefits of both optimize-then-discretize and discretize-then-optimize approaches.

Specifically, we establish the shape Fréchet differentiability of discrete (unfitted) bulk shape functionals using both the perturbation of the identity approach and direct perturbation of the level set representation. The latter approach is especially convenient for optimizing with respect to level set functions. Moreover, our Fréchet differentiability results hold for *any* polynomial degree used for the discrete level set representation of the domain. We illustrate our results with some numerical accuracy tests, a simple model (geometric) problem with known exact solution, as well as shape optimization of structural designs.

We also present some analysis of the Landau–de Gennes model for liquid crystals in an unfitted framework and derive a consistency estimate for a scalar-valued version of this PDE. These results will (eventually) form the foundation of an unfitted method for the Landau–de Gennes model.

Chapter 1. Introduction

Considerable work has been done on shape optimization with the following references giving a good overview [62, 38, 69, 39, 76, 66]. The main idea is to optimize (e.g. minimize) an objective functional over an admissible set of shapes or domains. Typically, the objective functional depends on the solution of a partial differential equation (PDE) over the domain to be optimized [74, 42], which gives a PDE-constrained, shape optimization problem. A classic example is finding the shape of a rigid body in a fluid flow that has minimum drag (i.e. that minimizes the viscous dissipation in the fluid velocity field around the body) [60, 61, 53, 34]. Other applications can be found in image processing [41, 23], microswimmers and fluids [77, 78, 48], and optimal (elastic) structures [19, 17].

For practical applications, one usually uses gradient-based optimization to find optimal shapes; thus, one has to calculate *shape derivatives* to obtain effective descent directions [38]. For the continuous problem, one can derive exact shape derivative formulas provided the domain and PDE-data are sufficiently smooth [22]. But these formulas depend on solutions of PDEs, which are almost never analytically tractable. Moreover, the domain geometry must be represented in a way that can be easily varied for optimization purposes. Hence, for real applications, numerical discretization of the PDE and geometry is necessary to make shape optimization problems tractable. A variety of numerical methods may be used for shape optimization, though finite element methods (FEM) are popular [43] because of their ability to handle complex geometry.

However, using FEMs with conforming meshes for the domain geometry introduces an issue for gradient-based optimization methods. The discrete objective functional now depends on the mesh vertex positions in a non-obvious way [5] and can be complicated to differentiate [29, 40] or requires automatic differentiation [46]. Essentially, the difficulty comes from the fact that perturbing the mesh (geometry) also perturbs the finite element space used for computing the PDE solution. The approach just described is called the *Discretize-then-Optimize* approach.

The alternative approach is called *Optimize-then-Discretize*. In this case, one derives the exact shape derivative formulas at the continuous level, then simply replaces all quantities with their discrete approximation [1]. Thus, computing the derivative is more straightforward than the other approach. Unfortunately, it suffers from *inconsistent gradients*, i.e. the discrete approximation of the shape derivative is **not** the exact derivative of the discrete objective functional. Hence, a gradient-based optimization method that uses these derivatives may get stuck and not reach a true optimum. In addition, one has to deform the mesh as the domain changes which introduces some challenges, such as avoiding mesh degeneracies and general remeshing of the domain [1]. Despite this, some success is enjoyed by this approach [45, 54], but the issues remain. See [33, 7] for a detailed discussion on the *Optimize-then-Discretize* versus *Discretize-then-Optimize* approaches.

Therefore, we propose an unfitted approach for shape optimization that avoids the above dichotomy. Our method uses discrete level set functions to represent the domain and an unfitted FEM for solving the PDEs. We show that, for bulk shape functionals, the exact, discrete shape derivative in terms of perturbing the domain's discrete level set function can be easily computed and, essentially, matches the continuous formula. Effectively, we take the discretize-then-optimize approach, but our formula is the same as that from the optimize-then-discretize approach (c.f. Sec. 5.5). Ergo, we gain the benefits of both approaches.

In [25], they consider shape optimization with extended FEM and level sets and apply finite differences (with respect to the level set) to the finite element stiffness matrix and load vector. However, this is a purely discretize-then-optimize approach and the computed shape derivative is not easy to interpret. In [24], they consider shape optimization with multi-meshes and they describe a method of mappings approach that yields a (seemingly) simple discrete shape derivative formula that is discretely consistent. However, they demonstrate that applying their formula to a Poisson problem results in a complicated formula involving many jump terms and special extension terms that are not easy to implement within their FEM framework. They then opt for a Hadamard formulation of the shape derivative, which is the optimize-then-discretize approach and gives gradients that are not consistent.

The closest reference to our work is [6], which derived similar level set shape derivative formulas to ours (c.f. our Theorem 5.16 to [6, Thm 5.1]). Nevertheless, there are two main differences with our work: (i) we are able to prove Fréchet differentiability of our formulas, whereas [6] only proves Gâteaux differentiability; (ii) we allow for discrete level set functions of arbitrary polynomial degree, but [6] only considers piecewise linear level set functions. We also emphasize that [6] assumes that the zero level set does not pass through any vertices of the mesh, which is related to our Assumption 4. It is notable that [6] also considers boundary functionals, which we do not, however the resulting discrete formulas are much more complicated than the continuous versions.

Some other related works are the following. In [18], they apply cutFEM techniques and level sets to shape optimization of elastic structures, but their formulation is of the optimize-then-discretize type only. In [14], they consider a Bernoulli free boundary problem, which can be posed as a shape optimization problem, and its approximation by cutFEM. Moreover, they *formally* compute discrete shape derivatives in the Gâteaux sense under some smoothness assumptions, including a boundary value correction method, and compare these to using continuous derivative formulas. Numerical experiments show that the various derivative formulas perform similarly with some issues of getting stuck on local minimizers.

Recently in [29], they computed the exact shape and topological derivative of discrete shape functionals, but their analysis was limited to piecewise linear level set functions. Our analysis allows for discrete level sets of arbitrary polynomial degree and yields formulas that are easier to interpret than in [29]. Furthermore, [9, 8] presents theoretical tools for shape optimization of sets defined via intersection.

The thesis is split into two main sections: (i) a section on shape optimization with unfitted finite element methods (Chapters 2-8); (ii) development of an unfitted method for simulating liquid crystals (Chapters 9-11).

The discussion on shape optimization is organized as follows. Chapter 2 presents a model problem, shape optimization with linear elasticity as the PDE constraint, to illustrate our shape derivative technique. Next, in Chapter 3, the discretization of the linear elasticity PDE is introduced along with an unfitted finite element framework. The analysis of the model problem: existence and uniqueness, well-conditioning, and consistency estimates are addressed in Chapter 4. Chapter 5 discusses the shape derivative and establishes the shape Fréchet differentiability of discrete bulk shape functionals. Moreover, the shape derivative is connected to the level set formulation and allows for *direct* perturbation of the level set function. In Chapter 6, the full shape optimization algorithm is described within a level set framework that allows for directly updating the level set function. Then, we give numerical results to demonstrate the method in Chapter 7 with concluding remarks in Chapter 8.

Additionally, in Chapters 9 and 10, we address the Landau–de Gennes model for liquid crystals in the unfitted finite element framework and discuss the analysis for a scalar-valued version: a modified Allen–Cahn PDE. Some concluding remarks are given in Chapter 11.

Chapter 2. Linear Elasticity PDE

We setup a classic example problem to illustrate our unfitted approach to shape optimization. Let $\Omega \subset \mathbb{R}^d$, for $d = 2$ or 3 with Lipschitz boundary $\partial\Omega := \overline{\Gamma_{\mathrm{D}}} \cup \overline{\Gamma_{\mathrm{N}}}$ such that $\Gamma_{\mathrm{D}} \cap \Gamma_{\mathrm{N}} = \emptyset$. We also denote the outward normal of Ω by $\boldsymbol{\nu}$. We consider the following linear elasticity equations with displacement field $\boldsymbol{u}(\boldsymbol{x})$:

$$\begin{aligned} -\nabla \cdot \boldsymbol{\sigma} = \boldsymbol{f}, \quad \boldsymbol{\sigma} = 2\mu\epsilon(\nabla \boldsymbol{u}) + \lambda \mathrm{tr}(\epsilon(\nabla \boldsymbol{u}))\mathbf{I}, \quad \text{in } \Omega \\ \boldsymbol{u} = \mathbf{0}, \quad \text{on } \Gamma_{\mathrm{D}}, \qquad \boldsymbol{\sigma}\boldsymbol{\nu} = \boldsymbol{g}_{\mathrm{N}} \quad \text{on } \Gamma_{\mathrm{N}}, \end{aligned} \tag{2.1}$$

where $\epsilon(\nabla \boldsymbol{u}) := \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$, μ and λ are Lamé parameters, and $\boldsymbol{\sigma}$ is the stress tensor. Additionally, $\boldsymbol{f}$ and $\boldsymbol{g}_{\mathrm{N}}$ are body and surface force densities, respectively. The term $\nabla \cdot \boldsymbol{\sigma}$ denotes taking the row-wise divergence on $\boldsymbol{\sigma}$. An example of a 2-D elastic domain Ω is given in Figure 2.1. The typical physical example we consider is a cantilever, with zero Dirichlet boundary conditions indicating that the cantilever is anchored along Γ_{D}.

The weak formulation of (2.1) is as follows. First, define the linear and bilinear forms:

$$\begin{aligned} \chi(\Omega; \boldsymbol{v}) &:= (\boldsymbol{f}, \boldsymbol{v})_{\Omega} + (\boldsymbol{g}_{\mathrm{N}}, \boldsymbol{v})_{\Gamma_{\mathrm{N}}}, \quad \forall \boldsymbol{v} \in H^1(\Omega), \\ a(\Omega; \boldsymbol{u}, \boldsymbol{v}) &:= 2\mu (\epsilon(\nabla \boldsymbol{u}), \epsilon(\nabla \boldsymbol{v}))_{\Omega} + \lambda (\nabla \cdot \boldsymbol{u}, \nabla \cdot \boldsymbol{v})_{\Omega}, \quad \forall \boldsymbol{u}, \boldsymbol{v} \in H^1(\Omega). \end{aligned} \tag{2.2}$$

Then, we seek the unique solution $\boldsymbol{u} \in V_{\mathrm{D}}(\Omega) := \{\boldsymbol{v} \in H^1(\Omega) : \boldsymbol{v}|_{\Gamma_{\mathrm{D}}} = \mathbf{0}\}$ such that

$$a(\Omega; \boldsymbol{u}, \boldsymbol{v}) = \chi(\Omega; \boldsymbol{v}) \qquad \forall \boldsymbol{v} \in V_{\mathrm{D}}(\Omega). \tag{2.3}$$

We will sometimes denote the solution to (2.3) by $\boldsymbol{u}(\Omega)$ to emphasize the dependence of the solution on the domain Ω.

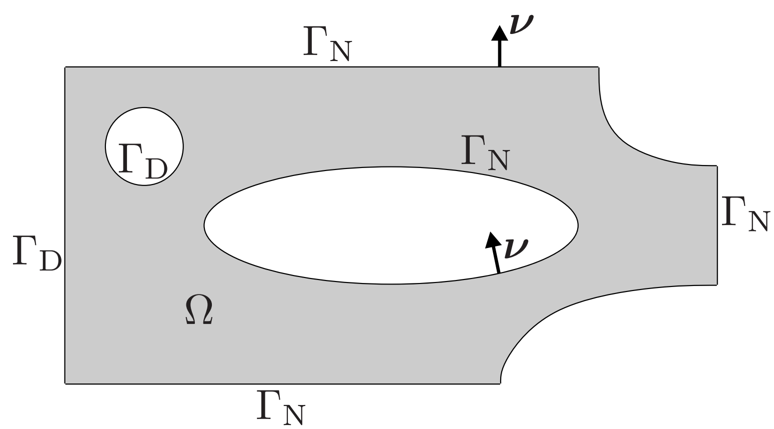


Figure 2.1. Diagram of 2-D domain representing a cantilever. The cantilever is anchored on the left and is hanging out freely to the right. Note that $\Gamma := \partial\Omega \equiv \Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{N}}$.

2.1. Minimization Problem

For any $\boldsymbol{v} \in V_{\mathrm{D}}$, let $J(\Omega; \boldsymbol{v})$ be a shape (cost) functional. Furthermore, let $\mathcal{A}$ be a set of admissible domains that accounts for some boundary constraints, regularity properties, etc., and consider the following minimization problem

$$J(\Omega_{\min}, \boldsymbol{u}(\Omega_{\min})) = \min_{\Omega \in \mathcal{A}} \min_{\boldsymbol{u} \in V_{\mathrm{D}}(\Omega)} J(\Omega; \boldsymbol{u}), \text{ subject to } \boldsymbol{u} \text{ uniquely solving (2.3) on } \Omega. \quad (2.4)$$

If $\mathcal{A}$ has some compactness properties, such as enforcing a bounded Lipschitz constant on the domains, see [1], then existence of a minimizer can be shown.

Proceeding formally, we rewrite the minimization problem using a Lagrangian to free the PDE-constraint, i.e. for any $\Omega \in \mathcal{A}$, define

$$L(\Omega; \boldsymbol{v}, \boldsymbol{q}) := J(\Omega; \boldsymbol{v}) - a(\Omega; \boldsymbol{v}, \boldsymbol{q}) + \chi(\Omega; \boldsymbol{q}), \quad \forall \boldsymbol{v}, \boldsymbol{q} \in H^1(\Omega), \quad (2.5)$$

and note that by (2.3) the following property holds

$$J(\Omega; \boldsymbol{u}(\Omega)) = L(\Omega; \boldsymbol{u}(\Omega), \boldsymbol{q}), \quad \forall \boldsymbol{q} \in V_{\mathrm{D}}(\Omega). \quad (2.6)$$

The Lagrangian framework allows us to characterize the minimizer in (2.4) as a saddle-point, i.e.

$$L\left(\bar{\Omega};\bar{\boldsymbol{u}},\bar{\boldsymbol{p}}\right)=\min_{\Omega\in\mathcal{A}}\ \min_{\boldsymbol{u}\in V_{\mathrm{D}}(\Omega)}\ \max_{\boldsymbol{q}\in V_{\mathrm{D}}(\Omega)} L\left(\Omega;\boldsymbol{v},\boldsymbol{q}\right), \tag{2.7}$$

for some $\bar{\Omega}\in\mathcal{A}$, $\bar{\boldsymbol{u}}\in V_{\mathrm{D}}$, and $\bar{\boldsymbol{p}}\in V_{\mathrm{D}}$. Assuming L is Fréchet differentiable, with $\delta_{\boldsymbol{q}}L\left(\Omega;\boldsymbol{v},\boldsymbol{q}\right)(\cdot)$, $\delta_{\boldsymbol{v}}L\left(\Omega;\boldsymbol{v},\boldsymbol{q}\right)(\cdot)$, and $\delta_{\Omega}L\left(\Omega;\boldsymbol{v},\boldsymbol{q}\right)(\cdot)$ denoting the Fréchet derivatives with respect to each argument, the following first order conditions must hold for $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{p}}$:

$$\begin{aligned}\delta_{\boldsymbol{q}}L\left(\bar{\Omega};\bar{\boldsymbol{u}},\bar{\boldsymbol{p}}\right)(\boldsymbol{z})=0,\quad\forall\boldsymbol{z}\in V_{\mathrm{D}}(\bar{\Omega}),\\ \delta_{\boldsymbol{v}}L\left(\bar{\Omega};\bar{\boldsymbol{u}},\bar{\boldsymbol{p}}\right)(\boldsymbol{w})=0,\quad\forall\boldsymbol{w}\in V_{\mathrm{D}}(\bar{\Omega}),\end{aligned} \tag{2.8}$$

which means that $\bar{\boldsymbol{u}}$ and $\bar{\boldsymbol{p}}$ solve the following variational problems

$$\begin{aligned}a\left(\bar{\Omega};\bar{\boldsymbol{u}},\boldsymbol{v}\right)=\chi\left(\bar{\Omega};\boldsymbol{v}\right),\ \forall\boldsymbol{v}\in V_{\mathrm{D}}(\bar{\Omega}),\\ a\left(\bar{\Omega};\boldsymbol{w},\bar{\boldsymbol{p}}\right)=\delta_{\boldsymbol{v}}J\left(\bar{\Omega};\bar{\boldsymbol{u}}\right)(\boldsymbol{w}),\ \forall\boldsymbol{w}\in V_{\mathrm{D}}(\bar{\Omega}).\end{aligned} \tag{2.9}$$

Thus, $\bar{\Omega}=\Omega_{\min}$, $\bar{\boldsymbol{u}}=\boldsymbol{u}(\Omega_{\min})$ solves (2.3) on $\Omega_{\min}$ and $\bar{\boldsymbol{p}}=\boldsymbol{p}(\Omega_{\min})$ solves an adjoint problem. In addition, we have the following first order condition for $\bar{\Omega}$:

$$\delta_{\Omega}L\left(\bar{\Omega};\bar{\boldsymbol{u}},\bar{\boldsymbol{p}}\right)(\boldsymbol{Y})=\delta_{\Omega}J\left(\Omega;\bar{\boldsymbol{u}}\right)(\boldsymbol{Y})-\delta_{\Omega}a\left(\Omega;\bar{\boldsymbol{u}},\bar{\boldsymbol{p}}\right)(\boldsymbol{Y})+\delta_{\Omega}\chi\left(\Omega;\bar{\boldsymbol{p}}\right)(\boldsymbol{Y})=0, \tag{2.10}$$

for all admissible *shape perturbations* $\boldsymbol{Y}$.

Note that, ultimately, we are after the derivative of the reduced functional $\mathcal{J}(\Omega):=J\left(\Omega;\boldsymbol{u}(\Omega)\right)$, where $\boldsymbol{u}(\Omega)$ solves (2.3). Indeed, we seek to compute the shape derivative of $\mathcal{J}(\Omega)$, so that we can perform gradient based optimization (see Section 6.2). This is given by the Correa-Seeger theorem [22, pg. 427]:

$$\delta_{\Omega}\mathcal{J}(\Omega)(\boldsymbol{Y})=\delta_{\Omega}L\left(\Omega;\bar{\boldsymbol{u}}(\Omega),\bar{\boldsymbol{p}}(\Omega)\right)(\boldsymbol{Y}), \tag{2.11}$$

for any admissible domain Ω.

As an example shape functional, we are interested in the so-called *compliance* functional χ, plus a penalty term on the volume of the domain:

$$J\left(\Omega;\boldsymbol{v}\right)=\chi\left(\Omega;\boldsymbol{v}\right)+a_0|\Omega|, \tag{2.12}$$

where χ is a sum of the work of the external forces acting on Ω (note: $a_0>0$). Nevertheless, our level set shape derivative formulas can be applied to other bulk shape functionals. Note that by using (2.12), the problem is self-adjoint and $\bar{\boldsymbol{p}}=\bar{\boldsymbol{u}}$.

Chapter 3. Unfitted Discretization

Our shape derivative technique takes full advantage of the framework of unfitted FEM, which uses level sets to represent the domain, as well as a Nitsche method and interface stabilization to yield a well-posed problem [15, 36, 12, 16, 50]. This section describes our discretization of the forward problem (2.3) (see also [37]).

3.1. Domain Representation with Level Sets

Let $\phi : \widehat{\mathfrak{D}} \to \mathbb{R}$ be a C^1 level set function, with $c^{-1} \geq |\nabla\phi| \geq c > 0$ on $\widehat{\mathfrak{D}}$, where $\widehat{\mathfrak{D}} \subset \mathbb{R}^d$ is a fixed, open, "hold-all," polygonal domain (e.g. a box) that we call the *design domain*. We represent the exact domain Ω by $\Omega = \{\boldsymbol{x} \in \widehat{\mathfrak{D}} : \phi(\boldsymbol{x}) < 0\}$ (see Figure 3.1), where the boundary of Ω partitions as

$$\partial\Omega = \widehat{\Gamma} \cup \Gamma, \quad \text{where} \quad \widehat{\Gamma} := \partial\widehat{\mathfrak{D}} \cap \overline{\Omega}, \quad \text{and} \quad \Gamma := \{\boldsymbol{x} \in \widehat{\mathfrak{D}} : \phi(\boldsymbol{x}) = 0\}. \tag{3.1}$$

Essentially, Γ is the free part of the domain that is being optimized. Note that $\phi \neq 0$ on $\widehat{\Gamma}$, except on $\overline{\widehat{\Gamma}} \cap \overline{\Gamma}$. This partitioning of the boundary will induce an analogous partitioning of the Dirichlet and Neumann boundaries, i.e.

$$\partial\Omega \equiv \left(\widehat{\Gamma}_{\mathrm{D}} \cup \Gamma_{\mathrm{D}}\right) \cup \left(\widehat{\Gamma}_{\mathrm{N}} \cup \Gamma_{\mathrm{N}}\right) \equiv \underbrace{\left(\widehat{\Gamma}_{\mathrm{D}} \cup \widehat{\Gamma}_{\mathrm{N}}\right)}_{=\widehat{\Gamma}} \cup \underbrace{\left(\Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{N}}\right)}_{=\Gamma}, \tag{3.2}$$

and similarly for the discrete boundaries (see below). The "hatted" boundaries will be *inactive*, while "unhatted" are *active*.

The discrete domain is represented by a discrete version of ϕ, denoted ϕ_h. To this end, let $\widehat{\mathcal{T}}_h = \{T\}$ be a conforming shape regular mesh of $\widehat{\mathfrak{D}}$, where all $T \in \widehat{\mathcal{T}}_h$ are treated as open sets, and define the space

$$\mathcal{B}_h = \{\phi_h \in W^{1,\infty}(\widehat{\mathfrak{D}}) : \phi_h|_T \in W^{2,\infty}(T), \ \forall T \in \widehat{\mathcal{T}}_h\}, \tag{3.3}$$

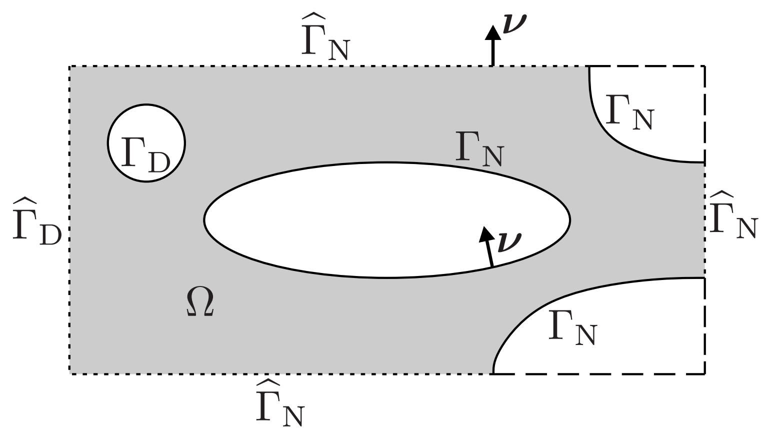


Figure 3.1. Diagram of the design domain. The outer design domain boundary $\partial\widehat{\mathfrak{D}}$ is indicated by the long and short dashed line, where the short dashed lines correspond to $\bar{\Omega} \cap \widehat{\Gamma}$; the solid boundaries indicate Γ.

with norm given by

$$\|\phi_h\|_{\mathcal{B}_h} := \|\phi_h\|_{W^{1,\infty}(\widehat{\mathfrak{D}})} + \max_{T\in\widehat{\mathcal{T}}_h} \|\nabla^2\phi_h\|_{L^\infty(T)}. \tag{3.4}$$

Then, we let $\phi_h \in \mathcal{B}_h$ and define the discrete domain $\Omega_h = \{\boldsymbol{x} \in \widehat{\mathfrak{D}} : \phi_h(\boldsymbol{x}) < 0\}$ with

$$\partial\Omega_h = \widehat{\Gamma}_h \cup \Gamma_h, \quad \widehat{\Gamma}_h := \partial\widehat{\mathfrak{D}} \cap \overline{\Omega_h}, \quad \text{and} \quad \Gamma_h := \{\boldsymbol{x} \in \widehat{\mathfrak{D}} : \phi_h(\boldsymbol{x}) = 0\}. \tag{3.5}$$

Again, we assume $c^{-1} \geq |\nabla\phi_h| \geq c > 0$ a.e. to guarantee Ω_h is well-defined and $\partial\Omega_h$ has dimension $d-1$. We also have an analogous partitioning of the discrete boundaries as in (3.2), i.e.

$$\partial\Omega_h \equiv \left(\widehat{\Gamma}_{h,\mathrm{D}} \cup \Gamma_{h,\mathrm{D}}\right) \cup \left(\widehat{\Gamma}_{h,\mathrm{N}} \cup \Gamma_{h,\mathrm{N}}\right) \equiv \left(\widehat{\Gamma}_{h,\mathrm{D}} \cup \widehat{\Gamma}_{h,\mathrm{N}}\right) \cup (\Gamma_{h,\mathrm{D}} \cup \Gamma_{h,\mathrm{N}}) = \widehat{\Gamma}_h \cup \Gamma_h. \tag{3.6}$$

In practice, we take $\phi_h \in B_h \subset \mathcal{B}_h$ to be a finite element function where B_h is a fixed, background (Lagrange) finite element space on $\widehat{\mathfrak{D}}$:

$$B_h = \{\boldsymbol{v}_h \in C^0(\widehat{\mathfrak{D}}) : \boldsymbol{v}_h|_T \in \mathcal{P}_k(T),\ \forall T \in \widehat{\mathcal{T}}_h\}, \quad \text{for some } k \geq 1. \tag{3.7}$$

Using level sets to represent geometries has a long history [57, 68], with some recent work on level set functions defined on unstructured meshes [4].

3.2. Subdomains and Meshes

For any given domain Ω (an open set with Lipschitz boundary), we approximate it by Ω_h which will be determined from an approximated level set function (as noted in (3.5)). Note that Ω will be changing due to shape optimization iterations. Let $\delta > 0$ be a layer thickness parameter (to be determined later) for extending domains, i.e. define the open set

$$\Omega_\delta = E_\delta(\Omega) := \operatorname{int}\{\boldsymbol{x} \in \widehat{\mathfrak{D}} : \operatorname{dist}(\boldsymbol{x}, \Omega) \leq \delta\}, \tag{3.8}$$

and $\Omega_{h,\delta} = E_\delta(\Omega_h)$. Note that $\Omega_0 \equiv \Omega$ and $\Omega_{h,0} = \Omega_h$. With this, we define the active mesh and corresponding domain (see Figure 3.2):

$$\begin{aligned} \mathcal{T}_\delta \equiv \mathcal{T}_{h,\delta} \equiv \mathcal{T}_{h,\delta}(\Omega_h) &= \{T \in \widehat{\mathcal{T}}_h : \Omega_{h,\delta} \cap T \neq \emptyset\}, \\ \mathfrak{D}_\delta \equiv \mathfrak{D}_{h,\delta} \equiv \mathfrak{D}_{h,\delta}(\Omega_h) &= \{\boldsymbol{x} \in T : T \in \mathcal{T}_{h,\delta}(\Omega_h)\}, \end{aligned} \tag{3.9}$$

where the discrete extended domains $\mathfrak{D}_\delta$ are jagged versions of $\Omega_{h,\delta}$.

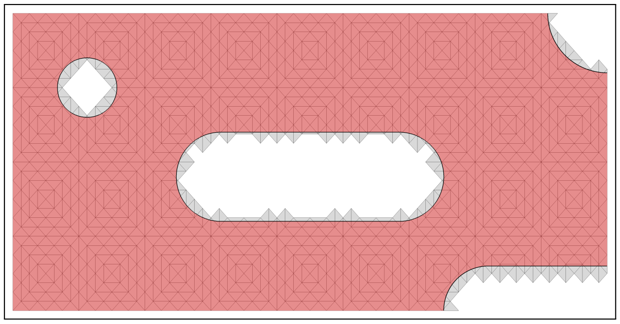
Next, we define the tubular (or shell region) that contains Γ_h (the active part):

$$\begin{aligned} \Sigma_\delta^\pm \equiv \Sigma_{h,\delta}^\pm \equiv \Sigma_{h,\delta}^\pm(\Gamma_h) &= \{\boldsymbol{x} \in \widehat{\mathfrak{D}} : \operatorname{dist}(\boldsymbol{x}, \Gamma_h) \leq \delta\}, \\ \Sigma_\delta^+ \equiv \Sigma_{h,\delta}^+ \equiv \Sigma_{h,\delta}^+(\Gamma_h) &= \{\boldsymbol{x} \in \widehat{\mathfrak{D}} \setminus \Omega_h : \operatorname{dist}(\boldsymbol{x}, \Gamma_h) \leq \delta\}, \end{aligned} \tag{3.10}$$

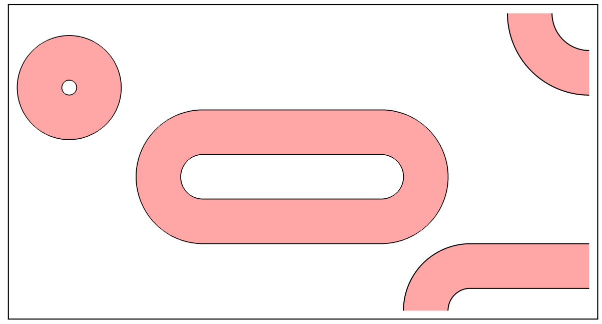
i.e. the shell regions always contain the zero level set. The corresponding meshes are (see Figure 3.2)

$$\begin{aligned} \mathcal{T}_{\Sigma^\pm} \equiv \mathcal{T}_{\Sigma_\delta^\pm}(\Gamma_h) &= \{T \in \widehat{\mathcal{T}}_h : T \cap \Sigma_\delta^\pm \neq \emptyset\}, \\ \mathcal{T}_{\Sigma^+} \equiv \mathcal{T}_{\Sigma_\delta^+}(\Gamma_h) &= \{T \in \widehat{\mathcal{T}}_h : T \cap \Sigma_\delta^+ \neq \emptyset\}. \end{aligned} \tag{3.11}$$

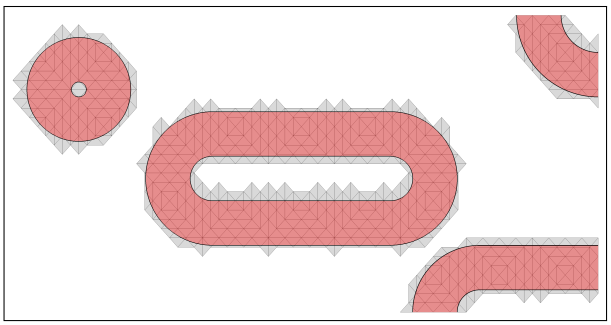
For simplicity, we assume that Γ_D and Γ_N lie on disconnected parts of Γ so that we



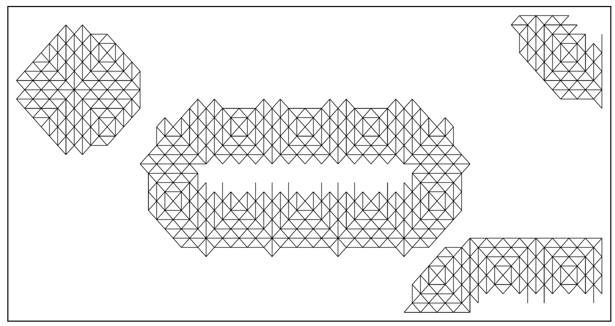
(a) The active mesh $\mathcal{T}_\delta$ depicted by the collection of elements above.



(b) In red, we have the shell region $\Sigma_\delta^\pm$ that surrounds the active boundary.



(c) The selection of elements, $\mathcal{T}_{\Sigma^\pm}$, around the shell region $\Sigma_\delta^\pm$.



(d) The facet selection $\mathcal{F}_{\Sigma^\pm}$ is depicted above.

Figure 3.2. Illustrations of subdomains.

have a clear decomposition:

$$\begin{aligned}&\Sigma^\pm_{h,\delta}(\Gamma_h) = \Sigma^\pm_{h,\delta,\mathrm{D}}(\Gamma_{h,\mathrm{D}}) \cup \Sigma^\pm_{h,\delta,\mathrm{N}}(\Gamma_{h,\mathrm{N}}), \quad \Sigma^+_{h,\delta}(\Gamma_h) = \Sigma^+_{h,\delta,\mathrm{D}}(\Gamma_{h,\mathrm{D}}) \cup \Sigma^+_{h,\delta,\mathrm{N}}(\Gamma_{h,\mathrm{N}}),\\ &\mathcal{T}_{\Sigma^\pm_\delta}(\Gamma_h) = \mathcal{T}_{\Sigma^\pm_{\delta,\mathrm{D}}} \cup \mathcal{T}_{\Sigma^\pm_{\delta,\mathrm{N}}}, \quad \mathcal{T}_{\Sigma^+_\delta}(\Gamma_h) = \mathcal{T}_{\Sigma^+_{\delta,\mathrm{D}}} \cup \mathcal{T}_{\Sigma^+_{\delta,\mathrm{N}}}.\end{aligned} \tag{3.12}$$

We also have the set of shell facets (see Figure 3.2):

$$\mathcal{F}_{\Sigma^\pm} \equiv \mathcal{F}_{\Sigma^\pm_\delta} = \{F \in \partial\mathcal{T}_{h,\delta} : F = \overline{T_1} \cap \overline{T_2},\ \text{for some } T_1 \in \mathcal{T}_{h,\delta}, T_2 \in \mathcal{T}_{\Sigma^\pm},\ \text{such that } T_1 \neq T_2\}, \tag{3.13}$$

where $\partial\mathcal{T}_{h,\delta} := \{\partial T : T \in \mathcal{T}_{h,\delta}\}$ denotes the set of all facets within the active mesh. Again we have the following decomposition: $\mathcal{F}_{\Sigma^\pm_\delta} = \mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}} \cup \mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{N}}}$. Note that the facets on the boundary of $\mathfrak{D}_{h,\delta}$ are *not* included in (3.13).

Remark 1. *One does not have to assume that Γ_D and Γ_N lie on disconnected parts of Γ. In this case, we alternatively define $\Sigma^\pm_{h,\delta,\mathrm{N}}(\Gamma_{h,\mathrm{N}})$ and $\Sigma^\pm_{h,\delta,\mathrm{D}}(\Gamma_{h,\mathrm{D}})$ as follows so that the two* *sets are disjoint:*

$$\begin{aligned} \Sigma^{\pm}_{\delta,\mathrm{D}} &\equiv \Sigma^{\pm}_{h,\delta,\mathrm{D}}(\Gamma_{h,\mathrm{D}}) := \{\boldsymbol{x} \in \widehat{\mathfrak{D}} : \mathrm{dist}\,(\boldsymbol{x}, \Gamma_{h,\mathrm{D}}) \leq \delta\}, \\ \Sigma^{\pm}_{\delta,\mathrm{N}} &\equiv \Sigma^{\pm}_{h,\delta,\mathrm{N}}(\Gamma_{h,\mathrm{N}}) := \Sigma^{\pm}_{\delta} \setminus \Sigma^{\pm}_{\delta,\mathrm{D}}. \end{aligned} \tag{3.14}$$

Similarly, the previous subdomain definitions can be redefined analogously for when Γ_{D} *and* Γ_{N} *are not disconnected. This will be necessary later for the continuity and coercivity of our bilinear form.*

3.3. The Finite Element Scheme

The background finite element space is based on B_h but with Dirichlet boundary conditions on $\widehat{\Gamma}_{h,\mathrm{D}}$ built-in:

$$\mathring{B}_h = B_h \cap \{\boldsymbol{v} \in H^1(\widehat{\mathfrak{D}}) : \boldsymbol{v}|_{\widehat{\Gamma}_{h,\mathrm{D}}} = 0\}. \tag{3.15}$$

With this, we have the restricted finite element space on $\mathfrak{D}_{h,\delta}$:

$$V_h \equiv V_h(\Omega_h) = \{\boldsymbol{v}_h \in C^0(\mathfrak{D}_{h,\delta}) : \boldsymbol{v}_h = \hat{\boldsymbol{v}}_h|_{\mathfrak{D}_{h,\delta}}, \text{ for some } \hat{\boldsymbol{v}}_h \in \mathring{B}_h\}, \tag{3.16}$$

i.e. $V_h = \mathring{B}_h|_{\mathfrak{D}_{h,\delta}}$.

The unfitted approach [37] for (2.3) requires special facet stabilization terms to ensure that the method is stable and that the condition number of the corresponding (finite dimensional) linear system does not depend on how elements are cut by the boundary. Given a facet $F = \overline{T_1} \cap \overline{T_2}$, with $T_1 \neq T_2$, let $\omega_F = T_1 \cup T_2$ be the local facet "patch." For any $\boldsymbol{u}, \boldsymbol{v} \in B_h$, define the local stabilization form, known as the "direct" version of the ghost penalty method as in [50]

$$s_{h,F}(\boldsymbol{u}, \boldsymbol{v}) := \int_{\omega_F} (\boldsymbol{u}_1 - \boldsymbol{u}_2) \cdot (\boldsymbol{v}_1 - \boldsymbol{v}_2) d\boldsymbol{x}, \tag{3.17}$$

where $\boldsymbol{u}_i = \mathcal{E}_{\mathcal{P}}\left(\boldsymbol{u}|_{T_i}\right)$ $(i = 1, 2)$, and similarly for $\boldsymbol{v}_i$, where $\mathcal{E}_{\mathcal{P}} : \mathcal{P}_k(T) \to \mathcal{P}_k(\mathbb{R}^d)$ is the obvious extension of a polynomial on an element T to all of $\mathbb{R}^d$ using its analytic formula. For the analysis, we also define (3.17) for arbitrary functions $\boldsymbol{u}, \boldsymbol{v} \in L^2(\widehat{\mathfrak{D}})$. Set $\boldsymbol{u}_i = \mathcal{E}_{\mathcal{P}}\left(\Pi_{T_i}\boldsymbol{u}|_{T_i}\right)$ $(i = 1, 2)$, where Π_{T_i} is the $L^2(T_i)$ projection onto $\mathcal{P}_k(T_i)$.

The global stabilization form, for a set of facets $\mathcal{F}$, is given by

$$s_h\left(\mathcal{F}; \boldsymbol{u}, \boldsymbol{v}\right) := \frac{1}{h^2} \sum_{F \in \mathcal{F}} s_{h,F}\left(\boldsymbol{u}, \boldsymbol{v}\right), \tag{3.18}$$

where $s_h\left(\mathcal{F}; \boldsymbol{u}, \boldsymbol{v}\right) \leq \left(s_h\left(\mathcal{F}; \boldsymbol{u}, \boldsymbol{u}\right)\right)^{1/2} \left(s_h\left(\mathcal{F}; \boldsymbol{v}, \boldsymbol{v}\right)\right)^{1/2}$ follows because $s_h\left(\mathcal{F}; \cdot, \cdot\right)$ is an inner product. Then, we introduce the following stabilized bilinear form:

$$a_h\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}\right) := a\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}\right) + \gamma_{\mathrm{s}} s_h(\mathcal{F}_{\Sigma^{\pm}_{\delta,D}}; \boldsymbol{u}, \boldsymbol{v}) + \gamma_{\mathrm{s}} h^2 s_h(\mathcal{F}_{\Sigma^{\pm}_{\delta,N}}; \boldsymbol{u}, \boldsymbol{v}), \tag{3.19}$$

where $\gamma_{\mathrm{s}} > 0$.

Next, we introduce the Nitsche stabilization technique for handling boundary conditions in our unfitted method. For all $\boldsymbol{u}, \boldsymbol{v} \in B_h$, define the following forms:

$$\begin{aligned} A_h\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}\right) &:= a_h\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}\right) - (\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{v})_{\Gamma_{h,D}} - (\boldsymbol{u}, \boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h)_{\Gamma_{h,D}} \\ &\quad + \gamma_{\mathrm{D}} h^{-1} b\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}\right) + \gamma_{\mathrm{N}} h (\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h)_{\Gamma_{h,N}} \\ b\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}\right) &:= 2\mu(\boldsymbol{u}, \boldsymbol{v})_{\Gamma_{h,D}} + \lambda(\boldsymbol{u} \cdot \boldsymbol{\nu}_h, \boldsymbol{v} \cdot \boldsymbol{\nu}_h)_{\Gamma_{h,D}} \\ \chi_h\left(\Omega_h; \boldsymbol{v}\right) &:= \chi\left(\Omega_h; \boldsymbol{v}\right) + \gamma_{\mathrm{N}} h (\boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h)_{\Gamma_{h,N}}, \end{aligned} \tag{3.20}$$

where $\gamma_{\mathrm{D}} > 0$, $\gamma_{\mathrm{N}} \geq 0$ are fixed coefficients. These forms are similarly defined on the exact domain Ω.

Our unfitted numerical scheme is as follows. Find $\boldsymbol{u}_h \in V_h(\Omega_h)$ such that

$$A_h\left(\Omega_h; \boldsymbol{u}_h, \boldsymbol{v}_h\right) = \chi_h\left(\Omega_h; \boldsymbol{v}_h\right) \qquad \forall \boldsymbol{v}_h \in V_h(\Omega_h), \tag{3.21}$$

where the Dirichlet condition on $\Gamma_{h,\mathrm{D}}$ is only penalized here. This scheme is a slight variation of the unfitted finite element method in [37] (see also [13]).

Let us (formally) verify the consistency of the scheme, though this is proved later in Section 4.4. For simplicity, we replace Ω_h by Ω and take the exact data $\boldsymbol{f}$ and $\boldsymbol{g}_\mathrm{N}$. Next, we substitute the exact solution $\boldsymbol{u}$ of (2.3) for $\boldsymbol{u}_h$ and integrate by parts

$$
\begin{aligned}
&(-\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{u}), \boldsymbol{v}_h)_{\Omega_h} + (\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}, \boldsymbol{v}_h)_{\Gamma_h} - (\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}, \boldsymbol{v}_h)_{\Gamma_{h,\mathrm{D}}} - (\boldsymbol{u}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu})_{\Gamma_{h,\mathrm{D}}} \\
&\quad + \gamma_\mathrm{D} h^{-1} b\,(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h) + \gamma_\mathrm{N} h\,(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu})_{\Gamma_{h,\mathrm{N}}} + (\text{stabiliz. forms}) \\
&\quad = (\boldsymbol{f}, \boldsymbol{v}_h)_{\Omega_h} + (\boldsymbol{g}_\mathrm{N}, \boldsymbol{v}_h)_{\Gamma_{h,\mathrm{N}}} + \gamma_\mathrm{N} h\,(\boldsymbol{g}_\mathrm{N}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu})_{\Gamma_{h,\mathrm{N}}},
\end{aligned}
\tag{3.22}
$$

for all $\boldsymbol{v}_h \in V_h(\Omega_h)$. Using the strong form (2.1) and rearranging, we get

$$
\begin{aligned}
&-(\boldsymbol{u}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu})_{\Gamma_{h,\mathrm{D}}} + \gamma_\mathrm{D} h^{-1} b\,(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h) \\
&\qquad + \gamma_\mathrm{N} h\,(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu} - \boldsymbol{g}_\mathrm{N}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu})_{\Gamma_{h,\mathrm{N}}} + (\text{stabiliz. forms}) = 0,
\end{aligned}
\tag{3.23}
$$

where the first three terms vanish by (2.1). The stabilization forms are not zero, but vanish as $h \to 0$ (see Prop. 4.4). Note: γ_N is allowed to be zero, but it may be useful to have in the case of other boundary conditions.

Chapter 4. Error Analysis for the Linear Elasticity PDE

We give a brief overview of the error analysis for the approximation of (2.3) with (3.21). To this end, we define some convenient norms:

$$\begin{aligned} \|\boldsymbol{v}\|_{a_h}^2 &:= a_h\left(\Omega_h; \boldsymbol{v}, \boldsymbol{v}\right), \quad \|\boldsymbol{v}\|_b^2 := b\left(\Omega_h; \boldsymbol{v}, \boldsymbol{v}\right), \\ |||\boldsymbol{v}|||_h^2 &:= \|\boldsymbol{v}\|_{a_h}^2 + h\|\boldsymbol{\sigma}(\boldsymbol{v})\|_{L^2(\Gamma_{h,\mathrm{D}})}^2 + \gamma_{\mathrm{N}} h\|\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h\|_{L^2(\Gamma_{h,\mathrm{N}})}^2 + h^{-1}\|\boldsymbol{v}\|_b^2, \end{aligned} \tag{4.1}$$

for all $\boldsymbol{v} \in H^2(\widehat{\mathfrak{D}}) \cup B_h$.

4.1. Inverse Estimates

In order to obtain some of these inverse estimates and to ensure coercivity of our bilinear form, we make a reasonable assumption, as in [50, Assumption 5.3], for a bound on the number facets that have been cut and a uniform bound (independent of h) on the number of paths that end on any interior element.

Assumption 1. *For every element $T \in \mathcal{T}_{\Sigma^+}$ there exists a path from $x \in T$ to a point within an interior element $y \in S \in \mathcal{T}_\delta \backslash \mathcal{T}_{\Sigma^+}$ and has the following properties: The number of facets that are cut by the path from x to y has a uniform bound of $K \lesssim (1 + \frac{\delta}{h})$ and the total number of paths that end in any interior element $S \in \mathcal{T}_\delta \backslash \mathcal{T}_{\Sigma^+}$ has a uniform bound, M, independent of h.*

This is a reasonable assumption as long as the interface Γ is smooth and sufficiently resolved by the mesh. We have the following useful inverse estimates.

Proposition 4.1. *Let $T_1 \in \mathcal{T}_{\Sigma^\pm}$ and $T_2 \in \mathcal{T}_\delta$ be such that $T_1 \neq T_2$ and $\bar{T}_1 \cap \bar{T}_2 = F \neq \emptyset$. Then for $\boldsymbol{u}$ with $\boldsymbol{u}|_{T_i} \in \mathcal{P}_m(T_i)$ for $i = 1, 2$, we have that*

$$\|\boldsymbol{u}\|_{L^2(T_1)}^2 \lesssim \|\boldsymbol{u}\|_{L^2(T_2)}^2 + s_{h,F}\left(\boldsymbol{u}, \boldsymbol{u}\right), \tag{4.2}$$

$$\|\nabla\boldsymbol{u}\|_{L^2(T_1)}^2 \lesssim \|\nabla\boldsymbol{u}\|_{L^2(T_2)}^2 + \frac{1}{h^2} s_{h,F}\left(\boldsymbol{u}, \boldsymbol{u}\right). \tag{4.3}$$

The proofs of (4.2) and (4.3) are given in Lemma 3.1 of [63] and in Lemma 5.2 of [50] respectively.

We also have the following extension estimates.

Proposition 4.2. *The following estimates hold for* $\boldsymbol{v} \in B_h$*:*

$$\|\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} \lesssim \|\boldsymbol{v}\|^2_{L^2(\Omega_h)} + Kh^2 s_h\left(\mathcal{F}_{\Sigma^{\pm}_{\delta}}; \boldsymbol{v}, \boldsymbol{v}\right), \tag{4.4}$$

$$\|\nabla\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} \lesssim \|\nabla\boldsymbol{v}\|^2_{L^2(\Omega_h)} + K s_h\left(\mathcal{F}_{\Sigma^{\pm}_{\delta}}; \boldsymbol{v}, \boldsymbol{v}\right), \tag{4.5}$$

$$2\mu\|\epsilon(\nabla\boldsymbol{v})\|^2_{L^2(\mathfrak{D}_\delta)} + \lambda\|\mathrm{tr}(\epsilon(\nabla\boldsymbol{v}))\|^2_{L^2(\mathfrak{D}_\delta)} \lesssim \|\nabla\boldsymbol{v}\|^2_{L^2(\Omega_h)} + K s_h\left(\mathcal{F}_{\Sigma^{\pm}_{\delta}}; \boldsymbol{v}, \boldsymbol{v}\right), \tag{4.6}$$

where $K \lesssim (1 + \frac{\delta}{h})$.

Proof. The proof uses (4.2) and (4.3) repeatedly. For every element $T \in \mathcal{T}_{\Sigma^+}$, we create a path from T to an interior element $T' \in \mathcal{T}_\delta \backslash \mathcal{T}_{\Sigma^+}$. The norm over T can be estimated by the norm over T' plus any facets that have been cut by our path. So, for (4.4), we have the following:

$$\begin{aligned}\|\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} &= \sum_{\forall T \in \mathcal{T}_\delta \backslash \mathcal{T}_{\Sigma+}} \|\boldsymbol{v}\|^2_{L^2(T)} + \sum_{\forall T \in \mathcal{T}_{\Sigma+}} \|\boldsymbol{v}\|^2_{L^2(T)} \\ &\lesssim \|\boldsymbol{v}\|^2_{L^2(\Omega_h)} + \sum_{\forall T \in \mathcal{T}_{\Sigma+}} \|\boldsymbol{v}\|^2_{L^2(T)},\end{aligned}$$

and now we use (4.2) repeatedly. Let us denote the path from any $T \in \mathcal{T}_{\Sigma^+}$ to an element $T' \in \mathcal{T}_\delta \backslash \mathcal{T}_{\Sigma^+}$ that has the desired properties in Assumption 1, by $p_T : [0,1] \to \widehat{\mathfrak{D}}$ and denote the collection of facets passed through by p_T by $\mathcal{F}_{p_T}$ having at most K facets in this collection. So then we get

$$\begin{aligned}\|\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} &\lesssim (M+1)\|\boldsymbol{v}\|^2_{L^2(\Omega_h)} + \sum_{\forall T \in \mathcal{T}_{\Sigma+}} \sum_{\forall F \in \mathcal{F}_{p_T}} s_{h,F}\left(\boldsymbol{v}, \boldsymbol{v}\right) \\ &\lesssim \|\boldsymbol{v}\|^2_{L^2(\Omega_h)} + Kh^2 s_h(\mathcal{F}_{\Sigma^{\pm}_{\delta}}; \boldsymbol{v}, \boldsymbol{v}),\end{aligned}$$

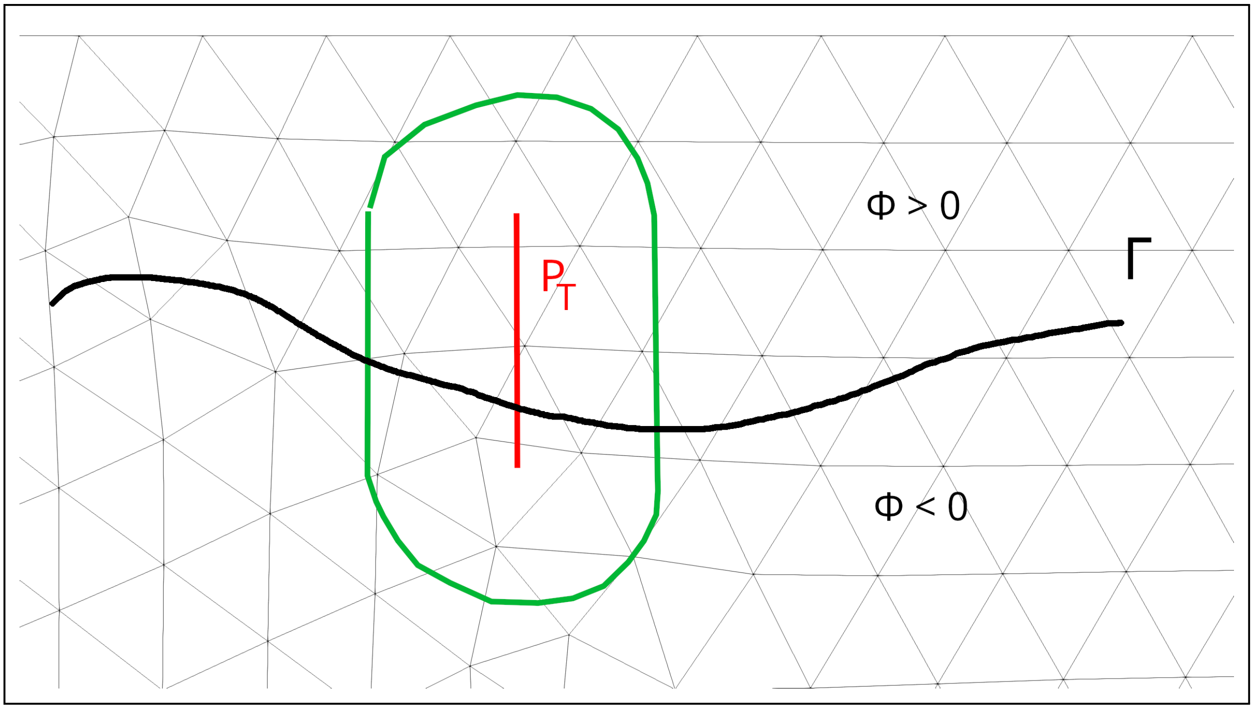


Figure 4.1. Example of a facet path, p_T, in red with a neighborhood of this path in green.

and the last line follows due to fact that $\mathcal{F}_{p_T} \subset \mathcal{F}_{\Sigma_\delta^\pm}$ and that any individual facet is passed through order $K \lesssim (1 + \frac{\delta}{h})$ number of times from paths p_T for all $T \in \mathcal{T}_{\Sigma^+}$. To understand this, we first consider how many facets any path p_T passes through. As shown in Figure 4.1, given any path p_T, we denote $\mathcal{O}_h(p_T)$ to be a neighborhood of p_T that has been extended by a distance of h. This guarantees that $\mathcal{O}_h(p_T)$ will contain all elements that p_T passes through. And due to the shape regularity of the mesh and the quasi-uniform mesh we can estimate K (the number of elements that intersect p_T) by taking the area of $\mathcal{O}_h(p_T)$ and dividing by the area of the smallest element. The length of p_T is at most δ, hence area of $\mathcal{O}_h(p_T)$ is at most $\pi h^2 + 2h\delta$ and the area of any element is of order h^2. Hence, $K \lesssim \frac{\pi h^2 + 2h\delta}{h^2} \lesssim (1 + \frac{\delta}{h})$.

As long as the mesh sufficiently resolves Γ, we should have the number of paths that pass through any individual facet is also of order K. Hence (4.4) follows, and the proof for (4.5) follows analogously. Now we consider (4.6):

$$
\begin{aligned}
2\mu\|\epsilon(\nabla \boldsymbol{v})\|^2_{L^2(\mathfrak{D}_\delta)} + \lambda\|\mathrm{tr}(\epsilon(\nabla \boldsymbol{v}))\|^2_{L^2(\mathfrak{D}_\delta)} &= \frac{1}{2}\mu\|\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T\|^2_{L^2(\mathfrak{D}_\delta)} + \frac{1}{4}\lambda\|\mathrm{tr}(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T)\|^2_{L^2(\mathfrak{D}_\delta)} \\
&\leq 2\mu\|\nabla \boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} + \lambda\|\mathrm{tr}(\nabla \boldsymbol{v})\|^2_{L^2(\mathfrak{D}_\delta)} \\
&\lesssim (2\mu+\lambda)\|\nabla \boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} \\
&\lesssim (2\mu+\lambda)\|\nabla \boldsymbol{v}\|^2_{L^2(\Omega_h)} + (2\mu+\lambda)Ks_h\left(\mathcal{F}_{\Sigma^\pm_\delta}; \boldsymbol{v}, \boldsymbol{v}\right),
\end{aligned}
$$

where we have used the inverse inequality (4.5). □

Corollary 4.3.

$$
\|\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,\mathrm{N}})} \lesssim \|\boldsymbol{v}\|^2_{L^2(\Omega_h)} + Kh^2 s_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}}; \boldsymbol{v}, \boldsymbol{v}\right), \quad (4.7)
$$

$$
\|\nabla\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,\mathrm{N}})} \lesssim \|\nabla\boldsymbol{v}\|^2_{L^2(\Omega_h)} + K s_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}}; \boldsymbol{v}, \boldsymbol{v}\right), \quad (4.8)
$$

$$
2\mu\|\epsilon(\nabla \boldsymbol{v})\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,\mathrm{N}})} + \lambda\|\mathrm{tr}(\epsilon(\nabla \boldsymbol{v}))\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,\mathrm{N}})} \lesssim \|\nabla\boldsymbol{v}\|^2_{L^2(\Omega_h)} + K s_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}}; \boldsymbol{v}, \boldsymbol{v}\right). \quad (4.9)
$$

Proof. The proof is similar to the proof of Prop. 4.2.

$$
\begin{aligned}
&2\mu\|\epsilon(\nabla \boldsymbol{v})\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,N})} + \lambda\|\mathrm{tr}(\epsilon(\nabla \boldsymbol{v}))\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,N})} \\
&\quad = \frac{1}{2}\mu\|\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,N})} + \frac{1}{4}\lambda\|\mathrm{tr}(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T)\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,N})} \\
&\quad \leq 2\mu\|\nabla \boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,N})} + \lambda\|\mathrm{tr}(\nabla \boldsymbol{v})\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,N})} \\
&\quad \leq (2\mu+\lambda)\|\nabla \boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,N})} \\
&\quad \lesssim (2\mu+\lambda)\|\nabla \boldsymbol{v}\|^2_{L^2(\Omega_h)} + (2\mu+\lambda)Ks_h(\mathcal{F}_{\Sigma^\pm_{\delta,D}}; \boldsymbol{v}, \boldsymbol{v}).
\end{aligned}
$$

Indeed, if we use $\mathfrak{D}_\delta\backslash\Sigma^\pm_{\delta,N}$ instead of $\mathfrak{D}_\delta$ we only end up with the facet stabilization term for facets belonging to $\mathcal{F}_{\Sigma^\pm_{\delta,D}}$. □

Remark 2. *Since we always assume that $|\widehat{\Gamma}_\mathrm{D}| > 0$, we have the classic Korn's inequality [20, Thm. 6.15-4]. Let $A \subset \widehat{\mathfrak{D}}$ be Lipschitz and assume that $\widehat{\Gamma}_\mathrm{D} \subset \partial A$. Then, there exists a* *constant* $C = C(A, \widehat{\Gamma}_{\mathrm{D}})$ *such that*

$$\|\boldsymbol{v}\|_{H^1(A)} \leq C\|\epsilon(\nabla \boldsymbol{v})\|_{L^2(A)}, \quad \text{for all } \boldsymbol{v} \in \mathring{B}_h. \tag{4.10}$$

Thus, for instance, one can bound the left-hand-side of (4.6) *below by* $\widetilde{C}\|\nabla \boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}$*, for some bounded constant* $\widetilde{C}$*.*

We will also need the following estimates for use in the a priori estimate.

Proposition 4.4. *For all* $\boldsymbol{v} \in H^k(\widehat{\mathfrak{D}})$ *we have the following estimate for the stabilization term:*

$$s_h\left(\mathcal{F}_{\Sigma_\delta^\pm}; \boldsymbol{v}, \boldsymbol{v}\right) \lesssim h^{2k}||\boldsymbol{u}||^2_{H^{k+1}(\mathfrak{D}_\delta)}, \tag{4.11}$$

and if $\mathcal{I}(\boldsymbol{v})$ *is the Lagrange (or Scott-Zhang) interpolant of* $\boldsymbol{v}$*, we also have*

$$s_h\left(\mathcal{F}_{\Sigma_\delta^\pm}; \boldsymbol{v} - \mathcal{I}(\boldsymbol{v}), \boldsymbol{v} - \mathcal{I}(\boldsymbol{v})\right) \lesssim h^{2k}||\boldsymbol{u}||^2_{H^{k+1}(\mathfrak{D}_\delta)}. \tag{4.12}$$

Proof. The proof can be found in [50, Lem. 5.8]. □

The following lemma is a generalization of [36, Lem. 4.2] (see also [37, eqn. (64)]).

Lemma 4.5. *Let* A *be a compact,* $C^{1,1}$ *domain in* $\mathbb{R}^d$*. Then, for any* $T \in \widehat{\mathcal{T}}_h$*, we have*

$$\|w\|^2_{L^2(\overline{T}\cap\partial A)} \leq C\left[(1+\kappa_0 h_T)\, h_T^{-1}\|w\|^2_{L^2(T)} + h_T\|\nabla w\|^2_{L^2(T)}\right], \quad \text{for all } w \in H^1(T), \tag{4.13}$$

where the constant C *is independent of* A *and* κ_0 *depends on* $\|\nabla^2 b_A\|_{L^\infty(\partial A)}$*, where* b_A *is the signed distance function of* A*.*

Proof. Set $S = \overline{T} \cap \partial A$ and note that $S \subset \partial T \cup \partial(T \cap A)$ by the following argument:

$$\begin{aligned} S = \overline{T} \cap \partial A &= (\partial T \cup T) \cap \partial A = (\partial T \cap \partial A) \cup (T \cap \partial A) \\ &\subset \partial T \cup [T \cap \partial A] \\ &\subset \partial T \cup \left[T \cap (\partial A \cap \overline{A^c})\right] \\ &\subset \partial T \cup \left[T \cap (A \cap \overline{A^c})\right] \\ &\subset \partial T \cup \left[(T \cap A) \cap (\overline{T^c} \cup \overline{A^c})\right] \\ &\subset \partial T \cup \left[\overline{(T \cap A)} \cap \overline{(T \cap A)^c}\right] \\ &= \partial T \cup \partial(T \cap A), \end{aligned} \tag{4.14}$$

where we have used the fact that $\partial B = \overline{B} \cap \overline{B^c}$. Define $T' = T \cap A$. We further decompose S into two subsets S_1 and S_2 where $S_1 = S \cap \partial T$ lies along ∂T and $S_2 = (S \cap \partial T') \setminus S_1$ lies entirely within the interior of T. By construction, $S_1 \cap S_2 = \emptyset$ and by (4.14) we have

$$\begin{aligned} S_1 \cup S_2 &= S \cap [\partial T \cup \partial T'] \\ &= S \cap [\partial T \cup \partial(T \cap A)] \\ &= S. \end{aligned} \tag{4.15}$$

Now we prove that $\|w\|^2_{L^2(S_i)}$ has the bound in (4.13) for $i = 1, 2$. Let $b_A : \mathbb{R}^d \to \mathbb{R}$ be the signed distance function of A, with $\mathrm{int}(A) = \{b_A(\boldsymbol{x}) < 0\}$. By [22, Ch. 5, Thm 4.3], and the compactness of A, there exists an open neighborhood $\mathcal{N}$ of ∂A such that $b_A \in C^{1,1}(\mathcal{N})$. By the classic Stein extension theorem, let $b : \mathbb{R}^d \to \mathbb{R}$ be a $C^{1,1}$ extension of $b_A|_{\mathcal{N}}$ to $\mathbb{R}^d$.

Next, let $\boldsymbol{F} : \widehat{T} \to T$ be an affine map from the unit diameter reference element $\widehat{T}$ to T, and note that $|\widehat{\nabla}\boldsymbol{F}| = O(h_T)$. Define $\widehat{A} = \boldsymbol{F}^{-1}(A)$, $\widehat{S} = \boldsymbol{F}^{-1}(S)$, $\widehat{T}' = \boldsymbol{F}^{-1}(T')$, $\widehat{S}_i = \boldsymbol{F}^{-1}(S_i)$, for $i = 1, 2$, and note that $\widehat{S} = \widehat{S}_1 \cup \widehat{S}_2$, $\widehat{S}_1 \cap \widehat{S}_2 = \emptyset$, $\widehat{S}_1 \subset \partial\widehat{T}$, and $\widehat{S}_2 \subset \partial\widehat{T}'$.

We also define $\hat{w} = w \circ \boldsymbol{F}$ and $\hat{b} = h_T^{-1} b \circ \boldsymbol{F}$, where $|\widehat{\nabla}\hat{b}| \leq O(1)$ everywhere, and note that $\widehat{\nabla}\hat{b}|_{\partial\widehat{A}} = \gamma_0 \hat{\boldsymbol{n}}_A$, where $0 < \gamma_0 = O(1)$ and $\hat{\boldsymbol{n}}_A$ is the (outward) unit normal of $\partial\widehat{A}$.

If $\widehat{S}_1 \neq \emptyset$, then let $\hat{\boldsymbol{n}}$ be the outward normal vector of $\partial\widehat{T}$ and note that

$$\int_{\partial\widehat{T}} \hat{\boldsymbol{n}} \cdot \widehat{\nabla}\hat{b}\, \hat{w}^2 dS = \pm\gamma_0 \int_{\widehat{S}_1} \hat{w}^2 dS + \int_{\partial\widehat{T}\setminus\widehat{S}_1} \hat{\boldsymbol{n}} \cdot \widehat{\nabla}\hat{b}\, \hat{w}^2 dS,$$

where the sign depends on the orientation of $\hat{\boldsymbol{n}}$. Using the divergence theorem, we have that

$$\int_{\partial\widehat{T}} \hat{\boldsymbol{n}} \cdot \widehat{\nabla}\hat{b}\, \hat{w}^2 dS = \int_{\widehat{T}} \widehat{\nabla} \cdot \left(\widehat{\nabla}\hat{b}\, \hat{w}^2\right) d\boldsymbol{x} = \int_{\widehat{T}} (\widehat{\Delta}\hat{b}) \hat{w}^2 d\boldsymbol{x} + 2\int_{\widehat{T}} \hat{w}\widehat{\nabla}\hat{b} \cdot \widehat{\nabla}\hat{w} d\boldsymbol{x}.$$

Combining, we get

$$\begin{aligned} \|\hat{w}\|^2_{L^2(\widehat{S}_1)} &\lesssim \|\widehat{\Delta}\hat{b}\|_{L^\infty(\widehat{T})} \|\hat{w}\|^2_{L^2(\widehat{T})} + \|\hat{w}\|_{L^2(\widehat{T})} \|\widehat{\nabla}\hat{w}\|_{L^2(\widehat{T})} + \|\hat{w}\|^2_{L^2(\partial\widehat{T})} \\ &\lesssim (1 + \|\widehat{\Delta}\hat{b}\|_{L^\infty(\widehat{T})}) \|\hat{w}\|^2_{L^2(\widehat{T})} + \|\widehat{\nabla}\hat{w}\|^2_{L^2(\widehat{T})}, \end{aligned} \tag{4.16}$$

where we used a standard trace inequality. If $\widehat{S}_1 = \emptyset$, then (4.16) trivially holds. Moreover, (4.16) holds with $\widehat{S}_1$ replaced with $\widehat{S}_2$. Summing the two inequalities, we get

$$\|\hat{w}\|^2_{L^2(\widehat{S})} \lesssim (1 + \|\widehat{\Delta}\hat{b}\|_{L^\infty(\widehat{T})}) \|\hat{w}\|^2_{L^2(\widehat{T})} + \|\widehat{\nabla}\hat{w}\|^2_{L^2(\widehat{T})}.$$

Mapping back to T, we obtain

$$\|w\|^2_{L^2(S)} \lesssim (1 + h_T \|\Delta b\|_{L^\infty(T)}) h_T^{-1} \|w\|^2_{L^2(T)} + h_T \|\nabla w\|^2_{L^2(T)},$$

where we note the scaling $|\widehat{\Delta}\hat{b}| \approx h_T |\Delta b|$, and that $|\Delta b|$ depends on the curvature of ∂A.

□

Proposition 4.6. *Given a domain Ω_h with Lipschitz boundary, we have the following standard trace and inverse estimates:*

$$\|\boldsymbol{v}\|^2_{L^2(\partial\Omega_h)} \lesssim \|\boldsymbol{v}\|_{L^2(\Omega_h)}\|\boldsymbol{v}\|_{H^1(\Omega_h)} \qquad \forall \boldsymbol{v} \in H^1(\Omega_h), \tag{4.17}$$

$$\|\boldsymbol{v}\|^2_{H^1(\mathfrak{D}_\delta)} \lesssim h^{-2}\|\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} \qquad \forall \boldsymbol{v} \in V_h(\mathfrak{D}_\delta), \tag{4.18}$$

$$h\|\nabla\boldsymbol{v}\|^2_{L^2(\Gamma_{h,\mathrm{D}})} \lesssim \|\nabla\boldsymbol{v}\|^2_{L^2(\Omega_h)} + K s_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}}; \boldsymbol{v}, \boldsymbol{v}\right) \qquad \forall \boldsymbol{v} \in V_h(\mathfrak{D}_\delta), \tag{4.19}$$

$$s_h\left(\mathcal{F}_{\Sigma^\pm}; \boldsymbol{v}, \boldsymbol{v}\right) \lesssim h^{-2}\|\boldsymbol{v}\|^2_{L^2(\mathcal{T}_{\Sigma^\pm})} \qquad \forall \boldsymbol{v} \in V_h(\mathfrak{D}_\delta). \tag{4.20}$$

Proof. The proofs of (4.17), (4.18), and can be found in Theorems 1.6.6, 4.5.11 of [11]. For (4.19), using Lemma 4.5 and inverse estimate (4.18) yields

$$\|\nabla\boldsymbol{v}\|^2_{L^2(\Gamma_{h,\mathrm{D}})} = \sum_{\substack{T\in\widehat{\mathcal{T}}_h \\ \overline{T}\cap\Gamma_{h,\mathrm{D}}\neq\emptyset}} \|\nabla\boldsymbol{v}\|^2_{L^2(\overline{T}\cap\Gamma_{h,\mathrm{D}})} \lesssim \sum_{\substack{T\in\widehat{\mathcal{T}}_h \\ \overline{T}\cap\Gamma_{h,\mathrm{D}}\neq\emptyset}} h^{-1}\|\nabla\boldsymbol{v}\|^2_{L^2(T)}.$$

Then, using (4.8), we get (4.19). We also note that the same argument also holds true for $\Gamma_{h,\mathrm{D}}$ replaced with Γ_h and $\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}}$ replaced with $\mathcal{F}_{\Sigma^\pm_\delta}$ due to (4.13) and (4.5).

The proof of (4.20) follows by approximating the L^2 norm over T_1 by the L^2 norm on an adjacent element T_2 which is justified due to the shape regularity of elements:

$$\begin{aligned} s_h\left(\mathcal{F}_{\Sigma^\pm}; \boldsymbol{v}, \boldsymbol{v}\right) &= \frac{1}{h^2}\sum_{F\in\mathcal{F}_{\Sigma^\pm}} \int_{\omega_F} (\boldsymbol{v}_1 - \boldsymbol{v}_2)^2 d\boldsymbol{x} \\ &\lesssim \frac{1}{h^2}\sum_{F\in\mathcal{F}_{\Sigma^\pm}} \int_{\omega_F} \boldsymbol{v}_1^2 + \boldsymbol{v}_2^2 d\boldsymbol{x} = \frac{1}{h^2}\sum_{F\in\mathcal{F}_{\Sigma^\pm}} \left[\int_{\omega_F} \boldsymbol{v}_1^2 d\boldsymbol{x} + \int_{\omega_F} \boldsymbol{v}_2^2 d\boldsymbol{x}\right], \end{aligned}$$

where we now use the shape regularity of the mesh to estimate the L^2 norm over T_1 and bound it by the L^2 norm over T_2 and vice versa, i.e.

$$\begin{aligned} s_h\left(\mathcal{F}_{\Sigma^\pm}; \boldsymbol{v}, \boldsymbol{v}\right) &\lesssim \frac{1}{h^2}\sum_{F\in\mathcal{F}_{\Sigma^\pm}} \left[\int_{T_1(F)} \boldsymbol{v}_1^2 d\boldsymbol{x} + \int_{T_2(F)} \boldsymbol{v}_2^2 d\boldsymbol{x}\right] \\ &\lesssim \sum_{F\in\mathcal{F}_{\Sigma^\pm}} \frac{1}{h^2}\int_{T_1(F)} \boldsymbol{v}_1^2 d\boldsymbol{x} = h^{-2}\|\boldsymbol{v}\|^2_{L^2(\mathcal{T}_{\Sigma^\pm})}. \end{aligned}$$

□

We first note the following estimates which can be found in [13, 37] and references therein.

Proposition 4.7. *The following inverse inequality and Poincaré estimate hold:*

$$|||\boldsymbol{v}|||_h \lesssim h^{-1}\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)} \qquad \forall \boldsymbol{v} \in V_h(\Omega_h), \tag{4.21}$$

$$\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)} \lesssim |||\boldsymbol{v}|||_h \qquad \forall \boldsymbol{v} \in V_h(\Omega_h). \tag{4.22}$$

Proof. Recall that $|||\boldsymbol{v}|||_h := \|\boldsymbol{v}\|_{a_h}^2 + h\|\boldsymbol{\sigma}(\boldsymbol{v})\|_{L^2(\Gamma_{h,\mathrm{D}})}^2 + \gamma_{\mathrm{N}} h\|\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h\|_{L^2(\Gamma_{h,\mathrm{N}})}^2 + h^{-1}\|\boldsymbol{v}\|_b^2$, so we proceed term-by-term. First,

$$\begin{aligned}
\|\boldsymbol{v}\|_{a_h}^2 &\equiv a\left(\Omega_h; \boldsymbol{v}, \boldsymbol{v}\right) + \gamma_{\mathrm{s}} s_h \left(\mathcal{F}_{\Sigma_{\delta,\mathrm{D}}^{\pm}}; \boldsymbol{v}, \boldsymbol{v}\right) + \gamma_{\mathrm{s}} h^2 s_h \left(\mathcal{F}_{\Sigma_{\delta,\mathrm{N}}^{\pm}}; \boldsymbol{v}, \boldsymbol{v}\right) \\
&\lesssim (\epsilon(\nabla \boldsymbol{v}), \epsilon(\nabla \boldsymbol{v}))_{\Omega_h} + (\nabla\cdot\boldsymbol{v}, \nabla\cdot\boldsymbol{v})_{\Omega_h} + h^{-2}\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}^2 + h^2 h^{-2}\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}^2 \\
&\lesssim \|\boldsymbol{v}\|_{H^1(\Omega_h)} + h^{-2}\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}^2 \lesssim h^{-2}\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}^2,
\end{aligned}$$

where we used the inverse inequalities (4.18) and (4.20). Next, using Proposition 4.6, we have

$$\begin{aligned}
h\|\boldsymbol{\sigma}(\boldsymbol{v})\|_{L^2(\Gamma_{h,\mathrm{D}})}^2 + \gamma_{\mathrm{N}} h\|\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h\|_{L^2(\Gamma_{h,\mathrm{N}})}^2 &\lesssim h\|\boldsymbol{\sigma}(\boldsymbol{v})\|_{L^2(\Gamma_h)}^2 \\
&= h\|2\mu(\epsilon(\nabla \boldsymbol{v})) + \lambda \mathrm{tr}(\epsilon(\nabla \boldsymbol{v}))I\|_{L^2(\Gamma_h)}^2 \\
&\lesssim h\|\nabla \boldsymbol{v}\|_{L^2(\Gamma_h)}^2 \\
&\lesssim \|\nabla \boldsymbol{v}\|_{L^2(\Omega_h)}^2 + K s_h\left(\mathcal{F}_{\Sigma_{\delta,\mathrm{D}}^{\pm}}; \boldsymbol{v}, \boldsymbol{v}\right) \\
&\lesssim h^{-2}\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}^2,
\end{aligned}$$

where we also used inequalities (4.18), (4.19), and (4.20). Next,

$$\begin{aligned}
h^{-1}\|\boldsymbol{v}\|_b^2 &\equiv h^{-1} 2\mu(\boldsymbol{v}, \boldsymbol{v})_{L^2(\Gamma_{h,\mathrm{D}})} + h^{-1}\lambda(\boldsymbol{v}\cdot\boldsymbol{\nu}, \boldsymbol{v}\cdot\boldsymbol{\nu})_{L^2(\Gamma_{h,\mathrm{D}})} \\
&\lesssim h^{-1}\|\boldsymbol{v}\|_{L^2(\Gamma_{h,\mathrm{D}})}^2 \lesssim h^{-1}\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}\|\boldsymbol{v}\|_{H^1(\mathfrak{D}_\delta)} \\
&\lesssim h^{-2}\|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}^2,
\end{aligned}$$

where we have used the trace inequality (4.17) and inverse inequality (4.18). Hence (4.21) is true. To show (4.22), we start with (4.4):

$$\begin{aligned}\|\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} &\lesssim \|\boldsymbol{v}\|^2_{L^2(\Omega_h)} + Kh^2 s_h\left(\mathcal{F}_{\Sigma^\pm_\delta};\boldsymbol{v},\boldsymbol{v}\right)\\ &\lesssim \|\boldsymbol{v}\|^2_{L^2(\Omega_h)} + Ks_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}};\boldsymbol{v},\boldsymbol{v}\right) + Kh^2 s_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{N}}};\boldsymbol{v},\boldsymbol{v}\right).\end{aligned}$$

Since $\boldsymbol{v} = \mathbf{0}$ on $\widehat{\Gamma}_{h,\mathrm{D}} \neq \emptyset$, it follows from the Poincaré inequality that

$$\begin{aligned}\|\boldsymbol{v}\|^2_{L^2(\mathfrak{D}_\delta)} &\lesssim \|\nabla\boldsymbol{v}\|^2_{L^2(\Omega_h)} + Ks_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}};\boldsymbol{v},\boldsymbol{v}\right) + Kh^2 s_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{N}}};\boldsymbol{v},\boldsymbol{v}\right)\\ &\lesssim 2\mu\|\epsilon(\nabla\boldsymbol{v})\|^2_{L^2(\Omega_h)} + \lambda\|\mathrm{tr}(\epsilon(\nabla\boldsymbol{v}))\|^2_{L^2(\Omega_h)} + Ks_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{D}}};\boldsymbol{v},\boldsymbol{v}\right) + Kh^2 s_h\left(\mathcal{F}_{\Sigma^\pm_{\delta,\mathrm{N}}};\boldsymbol{v},\boldsymbol{v}\right)\\ &\lesssim \|\boldsymbol{v}\|^2_{a_h} \lesssim |||\boldsymbol{v}|||^2_h.\end{aligned}$$

□

Proposition 4.8. *The bilinear form A_h is continuous and, for sufficiently large γ_D, coercive. Specifically, we have*

$$A_h\left(\Omega_h;\boldsymbol{u},\boldsymbol{v}\right) \lesssim |||\boldsymbol{u}|||_h\, |||\boldsymbol{v}|||_h\,, \qquad \forall \boldsymbol{u},\boldsymbol{v} \in V_h(\Omega_h), \tag{4.23}$$

$$|||\boldsymbol{v}|||^2_h \lesssim A_h\left(\Omega_h;\boldsymbol{v},\boldsymbol{v}\right), \qquad \forall \boldsymbol{v} \in V_h(\Omega_h). \tag{4.24}$$

Proof. Note that A_h defines an inner product on V_h. The continuity of A_h is trivial to show, so only the positive definiteness of A_h remains. So let $\boldsymbol{v} \in V_h$ with $\boldsymbol{v} \neq \mathbf{0}$ and note that we have the following:

$$\begin{aligned}|(\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h,\boldsymbol{v})_{\Gamma_{h,\mathrm{D}}}| &\le \Big(2\mu\|\epsilon(\nabla\boldsymbol{v})\|_{\Gamma_{h,\mathrm{D}}} + \lambda\|\mathrm{tr}(\epsilon(\nabla\boldsymbol{v}))\|_{\Gamma_{h,\mathrm{D}}}\Big)\|\boldsymbol{v}\|_b\\ &\lesssim \Big(2\mu\|\epsilon(\nabla\boldsymbol{v})\|^2_{\Gamma_{h,\mathrm{D}}} + \lambda\|\mathrm{tr}(\epsilon(\nabla\boldsymbol{v}))\|^2_{\Gamma_{h,\mathrm{D}}}\Big)^{1/2}\|\boldsymbol{v}\|_b\\ &\lesssim \frac{\delta h}{2}\Big(2\mu\|\epsilon(\nabla\boldsymbol{v})\|^2_{\Gamma_{h,\mathrm{D}}} + \lambda\|\mathrm{tr}(\epsilon(\nabla\boldsymbol{v}))\|^2_{\Gamma_{h,\mathrm{D}}}\Big) + \frac{1}{2\delta h}\|\boldsymbol{v}\|^2_b\\ &\cong \sum_{K\in\widehat{\mathcal{T}}_h}\frac{\delta h}{2}\Big(2\mu\|\epsilon(\nabla\boldsymbol{v})\|^2_{\Gamma_{h,\mathrm{D}}\cap K} + \lambda\|\mathrm{tr}(\epsilon(\nabla\boldsymbol{v}))\|^2_{\Gamma_{h,\mathrm{D}}\cap K}\Big) + \frac{1}{2\delta h}\|\boldsymbol{v}\|^2_b.\end{aligned}$$

Using the trace inequality from Lemma 4.5, we have

$$h\Big(2\mu\|\epsilon(\nabla \boldsymbol{v})\|^2_{\Gamma_{h,\mathrm{D}}\cap K}+\lambda\|\mathrm{tr}(\epsilon(\nabla \boldsymbol{v}))\|^2_{\Gamma_{h,\mathrm{D}}\cap K}\Big)\lesssim\Big(2\mu\|\epsilon(\nabla \boldsymbol{v})\|^2_{K}+\lambda\|\mathrm{tr}(\epsilon(\nabla \boldsymbol{v}))\|^2_{K}\Big).$$

Thus, we obtain:

$$\begin{aligned}|(\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h,\boldsymbol{v})_{\Gamma_{h,\mathrm{D}}}| &\lesssim \frac{\delta}{2}\Big(2\mu\|\epsilon(\nabla \boldsymbol{v})\|^2_{\mathcal{T}_{\Sigma^{\pm}_{\delta,\mathrm{D}}}}+\lambda\|\mathrm{tr}(\epsilon(\nabla \boldsymbol{v}))\|^2_{\mathcal{T}_{\Sigma^{\pm}_{\delta,\mathrm{D}}}}\Big)+\frac{1}{2\delta h}\|\boldsymbol{v}\|^2_b\\ &\lesssim \frac{\delta}{2}\Big(2\mu\|\epsilon(\nabla \boldsymbol{v})\|^2_{\mathfrak{D}_\delta\setminus\Sigma^{\pm}_{\delta,\mathrm{N}}}+\lambda\|\mathrm{tr}(\epsilon(\nabla \boldsymbol{v}))\|^2_{\mathfrak{D}_\delta\setminus\Sigma^{\pm}_{\delta,\mathrm{N}}}\Big)+\frac{1}{2\delta h}\|\boldsymbol{v}\|^2_b.\end{aligned}$$

And then using (4.9) we get the following:

$$|(\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h,\boldsymbol{v})_{\Gamma_{h,\mathrm{D}}}| \le C\frac{\delta}{2}\left[\|\nabla\boldsymbol{v}\|^2_{L^2(\Omega_h)}+Ks_h\left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{D}}};\boldsymbol{v},\boldsymbol{v}\right)\right]+C\frac{1}{2\delta h}\|\boldsymbol{v}\|^2_b.$$

Note that by definition of a_h we have $\frac{1}{2}\|\nabla\boldsymbol{v}\|^2_{L^2(\Omega_h)}+\gamma_{\mathrm{s}}s_h\left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{D}}};\boldsymbol{v},\boldsymbol{v}\right)\le a_h\left(\Omega_h;\boldsymbol{v},\boldsymbol{v}\right)$. Hence, by choosing $\delta=\min\{\frac{1}{4C},\frac{\gamma_{\mathrm{s}}}{2CK}\}$ we get

$$|(\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h,\boldsymbol{v})_{\Gamma_{h,\mathrm{D}}}| \le \frac{1}{4}a_h\left(\Omega_h;\boldsymbol{v},\boldsymbol{v}\right)+Ch^{-1}\|\boldsymbol{v}\|^2_b.$$

Therefore, upon choosing γ_{D} sufficiently large (independent of h), it follows that

$$\begin{aligned}A_h\left(\Omega_h;\boldsymbol{v},\boldsymbol{v}\right) &\ge \frac{1}{2}\|\boldsymbol{v}\|^2_{a_h}+(\gamma_{\mathrm{D}}-C)h^{-1}\|\boldsymbol{v}\|_b+\gamma_{\mathrm{N}}h\left(\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h,\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}}\\ &\gtrsim \|\boldsymbol{v}\|^2_{a_h}+h\|\boldsymbol{\sigma}(\boldsymbol{v})\|^2_{L^2(\Gamma_{h,\mathrm{D}})}+h^{-1}\|\boldsymbol{v}\|_b+\gamma_{\mathrm{N}}h\|\boldsymbol{\sigma}(\boldsymbol{v})\boldsymbol{\nu}_h\|^2_{L^2(\Gamma_{h,\mathrm{N}})}\cong|||\boldsymbol{v}|||^2_h,\end{aligned}\tag{4.25}$$

where we invoke the definition of $\|\cdot\|_{a_h}$, (4.19), and Korn's inequality (4.10). This establishes the coercivity of A_h. □

Theorem 4.9. *There exists a unique $\boldsymbol{u}_h\in V_h(\Omega_h)$ such that*

$$A_h\left(\Omega_h;\boldsymbol{u}_h,\boldsymbol{v}_h\right)=\chi_h\left(\Omega_h;\boldsymbol{v}_h\right)\qquad\forall\boldsymbol{v}_h\in V_h(\Omega_h).\tag{4.26}$$

Proof. Due to the fact that A_h is continuous and coercive from the previous lemma and that χ_h is a bounded linear functional, the proof follows directly from the Lax-Milgram Theorem. □

4.2. Conditioning of the Mass and Stiffness Matrix

Let $\{\varphi_i\}_{i=1}^N$ be the standard finite element basis of $V_h(\Omega_h)$ with N denoting the dimension of V_h. So then for any $\boldsymbol{v} \in V_h(\Omega_h)$ we can rewrite $\boldsymbol{v}$ as $\boldsymbol{v} = \sum_{i=1}^{N} \hat{v}_i \varphi_i$. We define the form $m_h(\boldsymbol{u}, \boldsymbol{v}) := (\boldsymbol{u}, \boldsymbol{v})_{\Omega_h^n} + s_h\left(\mathcal{F}_{\Sigma_\delta^\pm}; \boldsymbol{u}, \boldsymbol{v}\right)$ and then define the mass and stiffness matrices $\mathbf{M}$ and $\mathbf{A}$ as follows:

$$m_{ij} := m_h(\varphi_i, \varphi_j) \qquad \Longleftrightarrow \quad m_h(\boldsymbol{v}, \boldsymbol{w}) = (\mathbf{M}\hat{\boldsymbol{v}}, \hat{\boldsymbol{w}})_{\mathbb{R}^N}$$

$$a_{ij} := A_h\left(\Omega_h; \varphi_i, \varphi_j\right) \qquad \Longleftrightarrow \quad A_h\left(\Omega_h; \boldsymbol{v}, \boldsymbol{w}\right) = (\mathbf{A}\hat{\boldsymbol{v}}, \hat{\boldsymbol{w}})_{\mathbb{R}^N}$$

For all $\boldsymbol{v}, \boldsymbol{w} \in V_h(\Omega_h)$. We also recall a standard equivalence of norms estimate

$$h^d \|\hat{\boldsymbol{v}}\|_{\mathbb{R}^N}^2 \sim \|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)}^2. \tag{4.27}$$

We follow the proof of the theorem from [37] on the condition numbers of the mass and stiffness matrices:

Theorem 4.10. *The condition numbers of mass and stiffness matrices* $\boldsymbol{M}$ *and* $\boldsymbol{A}$ *satisfy the following estimates:*

$$\kappa(\boldsymbol{M}) \sim 1 \qquad \qquad \kappa(\boldsymbol{A}) \lesssim h^{-2}, \tag{4.28}$$

where the hidden constants are independent of h *and indepenent of the cut of the mesh.*

Proof. Note that we have the following

$$\begin{aligned}
(\mathbf{A}\hat{\boldsymbol{v}}, \hat{\boldsymbol{w}})_{\mathbb{R}^N} &= A_h\left(\Omega_h; \boldsymbol{v}, \boldsymbol{w}\right) \\
&\lesssim |||\boldsymbol{v}|||_h \, |||\boldsymbol{w}|||_h \\
&\lesssim h^{-2} \|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)} \|\boldsymbol{w}\|_{L^2(\mathfrak{D}_\delta)} \\
&\lesssim h^{d-2} \|\hat{\boldsymbol{v}}\|_{\mathbb{R}^N} \|\hat{\boldsymbol{w}}\|_{\mathbb{R}^N},
\end{aligned}$$

where we have used (4.23), (4.21), and (4.27). And so we have $(\mathbf{A}\hat{\boldsymbol{v}}, \hat{\boldsymbol{w}})_{\mathbb{R}^N} \lesssim h^{d-2}\|\hat{\boldsymbol{v}}\|_{\mathbb{R}^N}\|\hat{\boldsymbol{w}}\|_{\mathbb{R}^N}$ and by taking a supremum over all $\hat{\boldsymbol{w}}$ such that $\|\hat{\boldsymbol{w}}\|_{\mathbb{R}^N} = 1$ we obtain the fact that $\|\mathbf{A}\hat{\boldsymbol{v}}\|_{\mathbb{R}^N} \lesssim h^{d-2}\|\hat{\boldsymbol{v}}\|_{\mathbb{R}^N}$ which then implies $\|\mathbf{A}\|_{\mathbb{R}^N} \lesssim h^{d-2}$. Now to compute $\|\mathbf{A}^{-1}\|_{\mathbb{R}^N}$. Note that we have the following:

$$h^{d/2}\|\hat{\boldsymbol{v}}\|_{\mathbb{R}^N} \lesssim \|\boldsymbol{v}\|_{L^2(\mathfrak{D}_\delta)} \lesssim |||\boldsymbol{v}|||_h ,$$

Recall that by coercivity of A_h in (4.24) we have that $|||\boldsymbol{v}|||_h^2 \lesssim A_h(\Omega_h; \boldsymbol{v}, \boldsymbol{v})$ which implies

$$\begin{aligned} |||\boldsymbol{v}|||_h &\lesssim \frac{A_h(\Omega_h; \boldsymbol{v}, \boldsymbol{v})}{|||\boldsymbol{v}|||_h} \\ &\leq \sup_{\boldsymbol{w} \in V_h(\Omega_h)\setminus\{0\}} \frac{A_h(\Omega_h; \boldsymbol{v}, \boldsymbol{w})}{|||\boldsymbol{w}|||_h} \\ &= \sup_{\boldsymbol{w} \in V_h(\Omega_h)\setminus\{0\}} \frac{(\mathbf{A}\hat{\boldsymbol{v}}, \hat{\boldsymbol{w}})}{\|\hat{\boldsymbol{w}}\|_{\mathbb{R}^N}} \frac{\|\hat{\boldsymbol{w}}\|_{\mathbb{R}^N}}{|||\boldsymbol{w}|||_h} \\ &\lesssim \sup_{\boldsymbol{w} \in V_h(\Omega_h)\setminus\{0\}} h^{-d/2}\frac{(\mathbf{A}\hat{\boldsymbol{v}}, \hat{\boldsymbol{w}})}{\|\hat{\boldsymbol{w}}\|_{\mathbb{R}^N}}. \end{aligned}$$

Now then, we have the following:

$$h^d\|\hat{\boldsymbol{v}}\|_{\mathbb{R}^N} \lesssim \|\mathbf{A}\hat{\boldsymbol{v}}\|_{\mathbb{R}^N} \qquad \forall \hat{\boldsymbol{v}} \in \mathbb{R}^N.$$

Hence, by choosing $\hat{\boldsymbol{v}} = \mathbf{A}^{-1}\boldsymbol{w}$ we get that

$$\|\mathbf{A}^{-1}\hat{\boldsymbol{w}}\|_{\mathbb{R}^N} \lesssim h^{-d}\|\hat{\boldsymbol{w}}\|_{\mathbb{R}^N} \implies \|\mathbf{A}^{-1}\|_{\mathbb{R}^N} \lesssim h^{-d}.$$

So then it follows that $\kappa(A) = \|\mathbf{A}\|_{\mathbb{R}^N}\|\mathbf{A}^{-1}\|_{\mathbb{R}^N} \lesssim h^{-2}$.

The proof regarding the mass matrix can be proved in the same way but is slightly easier since we only need the equivalence of norms estimate (4.27) and continuity and coercivity properties of m_h □

4.3. Pseudo-Galerkin Orthogonality

We recall that our bilinear form $A_h(\Omega_h; \boldsymbol{u}, \boldsymbol{v})$ can be defined for functions $\boldsymbol{u}, \boldsymbol{v} \in H^1(\Omega_h)$. Moreover, we can extend the exact solution $\boldsymbol{u}$ on Ω to an open neighborhood $\mathfrak{D}_\delta$ that contains both Ω and Ω_h using the following bounded extension operator (see [11, Thm. 1.4.5]).

Theorem 4.11. *Suppose that Ω has a Lipschitz boundary and let $v \in W^{k,p}(\Omega)$. Then, there is an extension mapping $E : W^{k,p}(\Omega) \to W^{k,p}(\mathbb{R}^d)$ such that for all integers $k \geq 0$ and all $1 \leq p \leq \infty$, that satisfies*

$$E(v)|_\Omega = v \qquad \textit{and} \qquad \|E(v)\|_{W^{k,p}(\mathbb{R}^d)} \leq C\|v\|_{W^{k,p}(\Omega)},$$

where C is independent of v.

Now let $\boldsymbol{u} \in H^1(\Omega)$, with $\boldsymbol{u} = \boldsymbol{0}$ on $\Gamma_{\mathrm{D}} \cup \widehat{\Gamma}_{\mathrm{D}}$, solve (2.1) and assume $\boldsymbol{u} \equiv E(\boldsymbol{u})$ is extended to $H^1(\widehat{\mathfrak{D}})$ using Theorem 4.11. Now we also suitably extend $\boldsymbol{f}$ and $\boldsymbol{g}_{\mathrm{N}}$ so that $-\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{u}) = \boldsymbol{f}$ in Ω_h and $\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu} = \boldsymbol{g}_{\mathrm{N}}$ on $\Gamma_{h,\mathrm{N}}$. We also assume that $\boldsymbol{g}_{\mathrm{N}} = \boldsymbol{0}$ on $\widehat{\Gamma}_{h,\mathrm{N}}$. Then, $\boldsymbol{u}$ satisfies the following:

$$\begin{aligned}
(\boldsymbol{f}, \boldsymbol{v})_{\Omega_h} &= -(\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{u}), \boldsymbol{v})_{\Omega_h} \\
&= -(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{v})_{\partial\Omega_h} + (\boldsymbol{\sigma}(\boldsymbol{u}), \nabla \boldsymbol{v})_{\Omega_h} \\
&= -(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{v})_{\Gamma_{h,\mathrm{D}}} - (\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{v})_{\Gamma_{h,\mathrm{N}} \cup \widehat{\Gamma}_{h,\mathrm{N}}} + (\boldsymbol{\sigma}(\boldsymbol{u}), \nabla \boldsymbol{v})_{\Omega_h} \\
&= -(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{v})_{\Gamma_{h,\mathrm{D}}} - (\boldsymbol{g}_{\mathrm{N}}, \boldsymbol{v})_{\Gamma_{h,\mathrm{N}}} + a(\Omega_h; \boldsymbol{u}, \boldsymbol{v}) \\
(\boldsymbol{f}, \boldsymbol{v})_{\Omega_h} + (\boldsymbol{g}_{\mathrm{N}}, \boldsymbol{v})_{\Gamma_{h,\mathrm{N}}} &= a(\Omega_h; \boldsymbol{u}, \boldsymbol{v}) - (\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{v})_{\Gamma_{h,\mathrm{D}}} \\
\chi(\Omega_h; \boldsymbol{v}) &= a(\Omega_h; \boldsymbol{u}, \boldsymbol{v}) - (\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{v})_{\Gamma_{h,\mathrm{D}}}
\end{aligned} \tag{4.29}$$

where $\boldsymbol{v} \in \mathring{B}_h$ and $\boldsymbol{v} = \boldsymbol{0}$ on $\widehat{\Gamma}_{h,\mathrm{D}}$.

Proposition 4.12. *Let $\boldsymbol{R}(\boldsymbol{a},t) := \boldsymbol{a} + tY(\boldsymbol{a})$, for all t in a bounded, open interval I, and a.e. $\boldsymbol{a} \in \mathbb{R}^d$, where $Y \in [W^{1,\infty}(\mathbb{R}^d)]^d$. Assume that $\|Y\|_{W^{1,\infty}}$ is sufficiently small so that for all $t \in I$, $\nabla_{\boldsymbol{a}}\boldsymbol{R}(\boldsymbol{a},t)$ is a matrix with positive determinant and $|\nabla_{\boldsymbol{a}}\boldsymbol{R}(\boldsymbol{a},t)| = O(1)$, i.e. $\boldsymbol{R}(\cdot,t) : \mathbb{R}^d \to \mathbb{R}^d$ is a differentiable homeomorphism for all $t \in I$. Let $g \in L^1(\mathbb{R}^d)$ and define $q : \mathbb{R}^d \times I \to \mathbb{R}$ by $q(\boldsymbol{a},t) = g \circ \boldsymbol{R}(\boldsymbol{a},t)$. Then, $q \in L^1(\mathbb{R}^d \times I)$ and $\|q\|_{L^1(\mathbb{R}^d\times I)} \leq C|I| \cdot \|g\|_{L^1(\mathbb{R}^d)}$ for some bounded constant C.*

Proof. Define $\tilde{g} : \mathbb{R}^d \times I \to \mathbb{R}$ by $\tilde{g}(\boldsymbol{a},\tau) = g(\boldsymbol{a})$ for a.e. $\boldsymbol{a} \in \mathbb{R}^d$ and all $\tau \in I$. Clearly, $\tilde{g} \in L^1(\mathbb{R}^d \times I)$. Next, define $\boldsymbol{\Theta}(\boldsymbol{a},t) = (\boldsymbol{R}(\boldsymbol{a},t),t)$ and note that $\boldsymbol{\Theta} \in [W^{1,\infty}(\mathbb{R}^d \times I)]^{d+1}$. Moreover, we have that $\det(\nabla_{\boldsymbol{a},t}\boldsymbol{\Theta}(\boldsymbol{a},t)) = \det(\nabla_{\boldsymbol{a}}\boldsymbol{R}(\boldsymbol{a},t)) > 0$ for all $t \in I$. Thus, $\boldsymbol{\Theta} : \mathbb{R}^d \times I \to \mathbb{R}^d \times I$ is a differentiable homeomorphism.

Now, by change of variable, note that

$$\begin{aligned}\infty > |I| \cdot \|g\|_{L^1(\mathbb{R}^d)} = \int_{\mathbb{R}^d}\int_I |\tilde{g}(\boldsymbol{y},\tau)|d\tau d\boldsymbol{y} &= \int_{\mathbb{R}^d}\int_I |\tilde{g} \circ \boldsymbol{\Theta}(\boldsymbol{a},t)| \det(\nabla_{\boldsymbol{a},t}\boldsymbol{\Theta}(\boldsymbol{a},t))dtd\boldsymbol{a} \\ &= \int_{\mathbb{R}^d}\int_I |g \circ \boldsymbol{R}(\boldsymbol{a},t)| \det(\nabla_{\boldsymbol{a}}\boldsymbol{R}(\boldsymbol{a},t))dtd\boldsymbol{a},\end{aligned}$$

which means that $|g \circ \boldsymbol{R}| \det(\nabla_{\boldsymbol{a}}\boldsymbol{R})$ is in $L^1(\mathbb{R}^d \times I)$. Since $\det(\nabla_{\boldsymbol{a}}\boldsymbol{R}) \in L^\infty(\mathbb{R}^d \times I)$, then $q \equiv g \circ \boldsymbol{R} \in L^1(\mathbb{R}^d \times I)$ and $\|q\|_{L^1(\mathbb{R}^d\times I)} \leq C|I| \cdot \|g\|_{L^1(\mathbb{R}^d)}$. □

Corollary 4.13. *Let $\boldsymbol{R}(\boldsymbol{a},t)$ have the same function defined in Prop. 4.12. Now let $g \in L^p(\mathbb{R}^d)$, and define $q : \mathbb{R}^d \times I \to \mathbb{R}$ by $q(\boldsymbol{a},t) = g \circ \boldsymbol{R}(\boldsymbol{a},t)$. Then, $q \in L^p(\mathbb{R}^d \times I)$ and $\|q\|_{L^p(\mathbb{R}^d\times I)} \leq C|I|^{1/p}\|g\|_{L^p(\mathbb{R}^d)}$ for some bounded constant C.*

Corollary 4.14. *Let $\boldsymbol{R}(\boldsymbol{a},t)$ have the same function defined in Prop. 4.12. Now let $g \in H^1(\mathbb{R}^d)$ and let $\Gamma \subset \mathbb{R}^d$ be the Lipschitz boundary of a bounded set Ω, and define $q : \Gamma \times I \to \mathbb{R}$ by $q(\boldsymbol{a},t) = g \circ \boldsymbol{R}(\boldsymbol{a},t)$. Then, $q \in L^2(\Gamma \times I)$ and $\|q\|_{L^2(\Gamma\times I)} \leq C|I|^{1/2}\|g\|_{H^1(\mathbb{R}^d)}$ for some bounded constant C.*

Assumption 2. *We assume that the exact domain* Ω *is of class* C^{q+1}*, with* $q \geq 1$*, that* Ω_h *is the sub-zero level set of a discrete level set function* ϕ_h *having polynomial degree* q*, and that* Ω_h *approximates* Ω *to order* q *as described in* (4.30)*,* (4.31)*, and* (4.32)*. We also define our finite element space* V_h *to contain piecewise polynomials of up to order* q *and assume that* $\boldsymbol{g}_{\mathrm{N}} \in H^q(\widehat{\mathfrak{D}})$*,* $\boldsymbol{f} \in H^{q-1}(\widehat{\mathfrak{D}})$*.*

Assumption 2 implies that we have solution regularity $\boldsymbol{u} \in H^{q+1}(\Omega)$, and by the extension operator in Theorem 4.11, we consider $\boldsymbol{u}$ to be extended onto $\widehat{\mathfrak{D}}$ with $\boldsymbol{u} \in H^{q+1}(\widehat{\mathfrak{D}})$.

To proceed with our analysis, we use the same approach as in [32] and [50] in which we have an approximation of the discrete domain Ω_h, with the discrete level set function ϕ_h, satisfying

$$\operatorname{dist}(\Omega, \Omega_h) \lesssim h^{q+1}, \tag{4.30}$$

where $q \geq 1$ is the order of the geometry approximation (i.e. q is the polynomial degree of ϕ_h). In addition, we assume that there exists a mapping $\mathbf{\Phi}$ with the following properties:

$$\begin{aligned} &\mathbf{\Phi}(\Omega) = \Omega_h && \mathbf{\Phi}(\Omega_\delta) = \Omega_{h,\delta} \\ &\|\mathbf{\Phi} - \mathbf{id}\|_{L^\infty(\Omega_\delta)} \lesssim h^{q+1} && \|\nabla\mathbf{\Phi} - I\|_{L^\infty(\Omega_\delta)} \lesssim h^q \\ &\|\det(\nabla\mathbf{\Phi}) - 1\|_{L^\infty(\Omega_\delta)} \lesssim h^q, && \end{aligned} \tag{4.31}$$

where $\mathbf{\Phi}$ is a continuous well-defined map that is invertible for sufficiently small h, and $\boldsymbol{\nu} = \nabla\phi/|\nabla\phi|$ on Γ, $\boldsymbol{\nu}_h = \nabla\phi_h/|\nabla\phi_h|$ on Γ_h. Moreover, for surface elements, we note the following estimates from [32]

$$dS(\mathbf{\Phi}(\boldsymbol{a})) = \mu_h dS(\boldsymbol{a}), \quad \|\mu_h - 1\|_{L^\infty(\Gamma_h)} \lesssim h^q, \quad \|\boldsymbol{\nu} - \boldsymbol{\nu}_h\|_{L^\infty(\Gamma_h)} \lesssim h^q. \tag{4.32}$$

where dS_h (dS) represents the Lebesgue measure for Γ_h (Γ). We abuse notation and use

dS for either Γ or Γ_h depending on the context. The function μ_h is the Jacobian resulting from the change of variables for the surface integral.

The following basic result is needed to deal with the boundary stabilization terms coming from Nitsche's method (see Prop. 4.16).

Proposition 4.15. *Assume Ω, Ω_h satisfy the approximation properties* (4.31), (4.32). *Let $\Theta \subset \partial\Omega$ and Θ_h be its discrete approximation. Suppose $f \in H^1(\widehat{\mathfrak{D}})$ with $f = 0$ on Θ, and g_h is a piecewise polynomial function over $\widehat{\mathcal{T}}_h$. Then,*

$$(f, g_h)_{\Theta_h} \lesssim h^{(q+1)/2} \|f\|_{H^1(\widehat{\mathfrak{D}})} \cdot \|g_h\|_{L^2(\Theta_h)}, \tag{4.33}$$

$$(f, g_h)_{\Theta_h} \lesssim h^{q+1} \|\nabla f\|_{H^1(\widehat{\mathfrak{D}})} \cdot \|g_h\|_{L^2(\Theta_h)}, \quad \text{if } f \in H^2(\widehat{\mathfrak{D}}). \tag{4.34}$$

Proof. We start with

$$\begin{aligned} (f, g_h)_{\Theta_h} &= \int_{\Theta_h} f(x) g_h(x) dS \\ &= \int_{\Theta} (f \circ \mathbf{\Phi})(g_h \circ \mathbf{\Phi}) \mu_h dS \\ &= \int_{\Theta} (f \circ \mathbf{\Phi} - f)(g_h \circ \mathbf{\Phi}) \mu_h dS \\ &\lesssim \int_{\Theta} \Big| (f \circ \mathbf{\Phi} - f)(g_h \circ \mathbf{\Phi}) \Big| dS \\ &\lesssim \|f \circ \mathbf{\Phi} - f\|_{L^2(\Theta)} \cdot \|g_h \circ \mathbf{\Phi}\|_{L^2(\Theta)}, \end{aligned} \tag{4.35}$$

and note that $\|g_h \circ \mathbf{\Phi}\|_{L^2(\Theta)} \simeq \|g_h\|_{L^2(\Theta_h)}$. Next, we focus on the f term and use a refined trace estimate:

$$\|f \circ \mathbf{\Phi} - f\|^2_{L^2(\Theta)} \leq \|f \circ \mathbf{\Phi} - f\|^2_{L^2(\partial\Omega)} \lesssim \|f \circ \mathbf{\Phi} - f\|_{L^2(\Omega)} \|f \circ \mathbf{\Phi} - f\|_{H^1(\Omega)},$$

followed by

$$\begin{aligned}
\|f \circ \mathbf{\Phi} - f\|_{L^2(\Omega)} &\lesssim \left\| \int_0^1 \nabla f(\mathbf{id} + t(\mathbf{\Phi} - \mathbf{id})) \cdot (\mathbf{\Phi} - \mathbf{id}) dt \right\|_{L^2(\Omega)} \\
&\lesssim h^{q+1} \left\| \int_0^1 |\nabla f(\mathbf{id} + t(\mathbf{\Phi} - \mathbf{id}))| dt \right\|_{L^2(\Omega)} \\
&\lesssim h^{q+1} \|\nabla f\|_{L^2(\widehat{\mathfrak{D}})},
\end{aligned}$$

where we used Prop. 4.12 to view $\nabla f(\mathbf{id} + t(\mathbf{\Phi} - \mathbf{id}))$ as a function in $L^2(\widehat{\mathfrak{D}} \times [0,1])$ and apply the norm bound. Combining everything, we get (4.33).

Now, assume additional regularity of f, namely $f \in H^2(\widehat{\mathfrak{D}})$, and reconsider the f term in (4.35):

$$\begin{aligned}
\|f \circ \mathbf{\Phi} - f\|^2_{L^2(\Theta)} &= \left\| \int_0^1 \nabla f(\mathbf{id} + t(\mathbf{\Phi} - \mathbf{id})) \cdot (\mathbf{\Phi} - \mathbf{id}) dt \right\|^2_{L^2(\Theta)} \\
&\lesssim h^{2(q+1)} \left\| \int_0^1 |\nabla f(\mathbf{id} + t(\mathbf{\Phi} - \mathbf{id}))| dt \right\|^2_{L^2(\Theta)} \\
&\lesssim h^{2(q+1)} \int_\Theta \int_0^1 |\nabla f(\mathbf{id} + t(\mathbf{\Phi} - \mathbf{id}))|^2 dt dS \\
&\simeq h^{2(q+1)} \|\nabla f \circ \boldsymbol{R}\|^2_{L^2(\Theta \times [0,1])},
\end{aligned}$$

where $\boldsymbol{R}(\boldsymbol{a}, t) = \mathbf{id}(\boldsymbol{a}) + t(\mathbf{\Phi}(\boldsymbol{a}) - \mathbf{id}(\boldsymbol{a}))$. Then, we apply the trace inequality in Cor. 4.14 to obtain

$$\|f \circ \mathbf{\Phi} - f\|_{L^2(\Theta)} \lesssim h^{q+1} \|\nabla f\|_{H^1(\widehat{\mathfrak{D}})},$$

and combine with (4.35) to get (4.34). □

Proposition 4.16. *Let $q \geq 1$ be the order of approximation of Ω_h and assume Ω is C^{q+1}. Moreover, if $q = 1$, assume the (extended) exact solution $\boldsymbol{u}$ is in $H^2(\widehat{\mathfrak{D}})$ and $\boldsymbol{g}_{\mathrm{N}} \in H^1(\widehat{\mathfrak{D}})$;*

else, $\boldsymbol{u} \in H^3(\widehat{\mathfrak{D}})$ *and* $\boldsymbol{g}_{\mathrm{N}} \in H^2(\widehat{\mathfrak{D}})$. *Then, for all* $\boldsymbol{v}_h \in V_h(\Omega_h)$, *we have*

$$\begin{aligned} \gamma_{\mathrm{D}} h^{-1} b\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h\right) &\lesssim h^q \|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})} \|\boldsymbol{v}_h\|_{H^1(\Omega_h)}, \\ -\left(\boldsymbol{u}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{D}}} &\lesssim h^{q+1/2} \|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})} \|\!|\boldsymbol{v}_h|\!\|_h, \\ \gamma_{\mathrm{N}} h \left(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h - \boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} &\lesssim h^{q+1/2} \left[\|\boldsymbol{u}\|_{H^{\min\{q,2\}+1}(\widehat{\mathfrak{D}})} + \|\boldsymbol{g}_{\mathrm{N}}\|_{H^{\min\{q,2\}}(\widehat{\mathfrak{D}})}\right] \|\!|\boldsymbol{v}_h|\!\|_h. \end{aligned} \tag{4.36}$$

Proof. To derive the first line of (4.36), we use (4.34) and a trace estimate:

$$\begin{aligned} \gamma_{\mathrm{D}} h^{-1} b\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h\right) &= \gamma_{\mathrm{D}} h^{-1}\Big[2\mu(\boldsymbol{u}, \boldsymbol{v}_h)_{\Gamma_{h,\mathrm{D}}} + \lambda(\boldsymbol{u}\cdot\boldsymbol{\nu}_h, \boldsymbol{v}_h\cdot\boldsymbol{\nu}_h)_{\Gamma_{h,\mathrm{D}}}\Big] \\ &\lesssim \gamma_{\mathrm{D}} h^{-1}\Big[2\mu h^{q+1}\|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})} \cdot \|\boldsymbol{v}_h \circ \boldsymbol{\Phi}\|_{L^2(\Gamma_D)} \\ &\qquad + \lambda h^{q+1}\|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})} \cdot \|\boldsymbol{\nu}_h(\boldsymbol{v}_h\cdot\boldsymbol{\nu}_h)\circ\boldsymbol{\Phi}\|_{L^2(\Gamma_D)}\Big] \\ &\lesssim \gamma_{\mathrm{D}} h^q \|\boldsymbol{v}_h\|_{L^2(\Gamma_{h,\mathrm{D}})}\Big[2\mu\|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})} + \lambda\|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})}\Big] \lesssim h^q \|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})}\|\boldsymbol{v}_h\|_{H^1(\Omega_h)}. \end{aligned}$$

Next, we use (4.34) and the definition of $\|\!|\cdot|\!\|_h$ to obtain

$$-\left(\boldsymbol{u}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{D}}} \lesssim h^{q+1}\|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})}\|\boldsymbol{\sigma}(\boldsymbol{v}_h)\|_{L^2(\Gamma_{h,\mathrm{D}})} \lesssim h^{q+1/2}\|\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})} \|\!|\boldsymbol{v}_h|\!\|_h.$$

For the last estimate, note that

$$\left(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h - \boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} = \left(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu} - \boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} + \left(\boldsymbol{\sigma}(\boldsymbol{u})(\boldsymbol{\nu}_h - \boldsymbol{\nu}), \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}},$$

and estimating the second term with $\|\boldsymbol{\nu}_h - \boldsymbol{\nu}\|_{L^\infty(\Gamma_h)} \lesssim h^q$ gives

$$\begin{aligned} \gamma_{\mathrm{N}}\left(\boldsymbol{\sigma}(\boldsymbol{u})(\boldsymbol{\nu}_h - \boldsymbol{\nu}), \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} &\lesssim h^q\|\boldsymbol{\sigma}(\boldsymbol{u})\|_{L^2(\Gamma_{h,\mathrm{N}})}\gamma_{\mathrm{N}}\|\boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\|_{L^2(\Gamma_{h,\mathrm{N}})} \\ &\lesssim h^{q-1/2}\|\nabla\boldsymbol{u}\|_{H^1(\Omega_h)} \|\!|\boldsymbol{v}_h|\!\|_h. \end{aligned}$$

Now, we focus on the other term and first assume $q \geq 2$ and note that $\boldsymbol{u} \in H^3(\widehat{\mathfrak{D}})$ and $\boldsymbol{g}_{\mathrm{N}} \in H^2(\widehat{\mathfrak{D}})$. Again, we use (4.34) and the definition of $\|\!|\cdot|\!\|_h$ to get

$$\begin{aligned} \gamma_{\mathrm{N}}\left(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu} - \boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} &\lesssim h^{q+1}\|\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu} - \boldsymbol{g}_{\mathrm{N}}\|_{H^2(\widehat{\mathfrak{D}})}\gamma_{\mathrm{N}}\|\boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\|_{L^2(\Gamma_{h,\mathrm{N}})} \\ &\lesssim h^{q+1/2}\left[\|\nabla\boldsymbol{u}\|_{H^2(\widehat{\mathfrak{D}})} + \|\boldsymbol{g}_{\mathrm{N}}\|_{H^2(\widehat{\mathfrak{D}})}\right] \|\!|\boldsymbol{v}_h|\!\|_h. \end{aligned}$$

On the other hand, if $q = 1$, then we have the following estimate due to (4.33):

$$\begin{aligned}\gamma_{\mathrm{N}} \left(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu} - \boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} &\lesssim h \|\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu} - \boldsymbol{g}_{\mathrm{N}}\|_{H^1(\widehat{\mathfrak{D}})} \gamma_{\mathrm{N}} \|\boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\|_{L^2(\Gamma_{h,\mathrm{N}})} \\ &\lesssim h^{1/2} \left[\|\nabla \boldsymbol{u}\|_{H^1(\widehat{\mathfrak{D}})} + \|\boldsymbol{g}_{\mathrm{N}}\|_{H^1(\widehat{\mathfrak{D}})}\right] |||\boldsymbol{v}_h|||_h .\end{aligned}$$

Combining everything gives the last line of (4.36). □

4.4. A Priori Estimate

Since (4.29) is satisfied for all $\boldsymbol{v} \in \mathring{B}_h$, it follows that we can choose $\boldsymbol{v} = \boldsymbol{v}_h \in V_h(\Omega_h)$ so that we have

$$\begin{aligned}A_h\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h\right) = \chi_h\left(\Omega_h; \boldsymbol{v}_h\right) &- \left(\boldsymbol{u}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{D}}} + \gamma_{\mathrm{D}} h^{-1} b\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h\right) \\ &+ \gamma_{\mathrm{N}} h \left(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} - \gamma_{\mathrm{N}} h \left(\boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} \\ &+ \gamma_{\mathrm{s}} s_h \left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{D}}}; \boldsymbol{u}, \boldsymbol{v}_h\right) + \gamma_{\mathrm{s}} h^2 s_h \left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{N}}}; \boldsymbol{u}, \boldsymbol{v}_h\right) \quad \forall \boldsymbol{v}_h \in V_h(\Omega_h).\end{aligned} \tag{4.37}$$

Then, subtracting (3.21) we get the following pseudo Galerkin orthogonality property $\forall \boldsymbol{v}_h \in V_h(\Omega_h)$:

$$\begin{aligned}&A_h\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h\right) - A_h\left(\Omega_h; \boldsymbol{u}_h, \boldsymbol{v}_h\right) \\ &\quad = -\left(\boldsymbol{u}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{D}}} + \gamma_{\mathrm{D}} h^{-1} b\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h\right) + \gamma_{\mathrm{N}} h \left(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} \\ &\qquad - \gamma_{\mathrm{N}} h \left(\boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} + \gamma_{\mathrm{s}} s_h \left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{D}}}; \boldsymbol{u}, \boldsymbol{v}_h\right) + \gamma_{\mathrm{s}} h^2 s_h \left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{N}}}; \boldsymbol{u}, \boldsymbol{v}_h\right) \\ &\quad = -\left(\boldsymbol{u}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{D}}} + \gamma_{\mathrm{D}} h^{-1} b\left(\Omega_h; \boldsymbol{u}, \boldsymbol{v}_h\right) + \gamma_{\mathrm{N}} h \left(\boldsymbol{\sigma}(\boldsymbol{u})\boldsymbol{\nu}_h, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} \\ &\qquad - \gamma_{\mathrm{N}} h \left(\boldsymbol{g}_{\mathrm{N}}, \boldsymbol{\sigma}(\boldsymbol{v}_h)\boldsymbol{\nu}_h\right)_{\Gamma_{h,\mathrm{N}}} + \gamma_{\mathrm{s}} s_h \left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{D}}}; \boldsymbol{u}, \boldsymbol{v}_h\right) + \gamma_{\mathrm{s}} h^2 s_h \left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{N}}}; \boldsymbol{u}, \boldsymbol{v}_h\right) \\ &\quad \lesssim \gamma_{\mathrm{s}} s_h \left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{D}}}; \boldsymbol{u}, \boldsymbol{v}_h\right) + \gamma_{\mathrm{s}} h^2 s_h \left(\mathcal{F}_{\Sigma^{\pm}_{\delta,\mathrm{N}}}; \boldsymbol{u}, \boldsymbol{v}_h\right) \\ &\qquad + h^q \left[\|\boldsymbol{u}\|_{H^{\min\{q,2\}+1}(\widehat{\mathfrak{D}})} + \|\boldsymbol{g}_{\mathrm{N}}\|_{H^{\min\{q,2\}}(\widehat{\mathfrak{D}})}\right] |||\boldsymbol{v}_h|||_h ,\end{aligned} \tag{4.38}$$

where we have used (4.36) in the last line.

We first review a basic interpolation result [11]. Recall $\mathfrak{D}_\delta$ from (3.9) and assume $\delta > 0$ is large enough so that $\mathfrak{D}_\delta$ contains both Ω and Ω_h. Let $\pi_{h,SZ} : H^1(\mathfrak{D}_\delta) \to V_h(\Omega_h)$

be the Scott-Zhang interpolation operator and define $\pi_h : H^1(\Omega) \ni u \mapsto \pi_{h,SZ}E(u) \in V_h(\Omega_h)$, using the bounded extension operator from Theorem 4.11. For the remainder of this section, we abuse notation and write $\boldsymbol{u} \equiv E(\boldsymbol{u})$.

Proposition 4.17. *For all integers m, s, such that $0 \leq m \leq s \leq q+1$, where q is the polynomial degree of V_h, and $k \leq q$, we have*

$$\|\boldsymbol{u} - \pi_h \boldsymbol{u}\|_{H^m(\mathfrak{D}_\delta)} \lesssim h^{s-m} \|\boldsymbol{u}\|_{H^s(\Omega)},$$

$$|||\boldsymbol{u} - \pi_h \boldsymbol{u}|||_h \lesssim h^k \|\boldsymbol{u}\|_{H^{k+1}(\Omega)}.$$

From this, one can derive the following error estimate.

Theorem 4.18. *Let $\boldsymbol{u} \in H^{k+1}(\widehat{\mathfrak{D}})$ be the extended solution of* (2.1) *on Ω to $\widehat{\mathfrak{D}}$, and let $\boldsymbol{u}_h \in V_h(\Omega_h)$ be the finite element approximation defined in* (3.21) *with $q = k$. Then, the following a priori estimates hold*

$$\begin{aligned} |||\boldsymbol{u} - \boldsymbol{u}_h|||_h &\lesssim h^k \left[\|\boldsymbol{u}\|_{H^{k+1}(\Omega)} + \|\boldsymbol{g}_{\mathrm{N}}\|_{H^{\min\{k,2\}}(\widehat{\mathfrak{D}})} \right], \\ \|\boldsymbol{u} - \boldsymbol{u}_h\|_{L^2(\Omega)} &\lesssim h^{k+1} \left[\|\boldsymbol{u}\|_{H^{k+1}(\Omega)} + \|\boldsymbol{g}_{\mathrm{N}}\|_{H^{\min\{k,2\}}(\widehat{\mathfrak{D}})} \right], \end{aligned} \tag{4.39}$$

where by some standard a priori PDE estimates we also have $\|\boldsymbol{u}\|_{H^{k+1}(\Omega)} \lesssim ||\boldsymbol{f}||_{H^{k-1}(\Omega)} + \|\boldsymbol{g}_{\mathrm{N}}\|_{H^k(\Omega)}$ [26].

Proof. By the triangle inequality and our interpolation estimate, we have

$$|||\boldsymbol{u} - \boldsymbol{u}_h|||_h \lesssim |||\boldsymbol{u} - \pi_h \boldsymbol{u}|||_h + |||\pi_h \boldsymbol{u} - \boldsymbol{u}_h|||_h \lesssim h^k \|\boldsymbol{u}\|_{H^{k+1}(\Omega)} + |||\pi_h \boldsymbol{u} - \boldsymbol{u}_h|||_h . \tag{4.40}$$

Now we deal with the second term above using the coercivity of A_h:

$$
\begin{aligned}
\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h^2 &\lesssim A_h\left(\Omega_h ; \pi_h \boldsymbol{u}-\boldsymbol{u}_h, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right) \\
&= A_h\left(\Omega_h ; \pi_h \boldsymbol{u}-\boldsymbol{u}, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right)+A_h\left(\Omega_h ; \boldsymbol{u}-\boldsymbol{u}_h, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right) \\
&\lesssim \left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}\right|\!\right|\!\right|_h \cdot \left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h+A_h\left(\Omega_h ; \boldsymbol{u}-\boldsymbol{u}_h, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right) \\
&\lesssim \frac{1}{2 \epsilon}\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}\right|\!\right|\!\right|_h^2+\frac{\epsilon}{2}\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h^2+A_h\left(\Omega_h ; \boldsymbol{u}-\boldsymbol{u}_h, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right),
\end{aligned}
$$

where we used a weighted Young's inequality. Then, by choosing ϵ appropriately and reordering terms, we obtain $\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h^2 \lesssim \left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}\right|\!\right|\!\right|_h^2+A_h\left(\Omega_h ; \boldsymbol{u}-\boldsymbol{u}_h, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right)$.

Next, we use the pseudo-Galerkin orthogonality property (4.38) and note the geometry approximation of Ω is order $q=k$. Thus, we get the following:

$$
\begin{aligned}
\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h^2 &\lesssim \left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}\right|\!\right|\!\right|_h^2+A_h\left(\Omega_h ; \boldsymbol{u}-\boldsymbol{u}_h, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right) \\
&\lesssim \left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}\right|\!\right|\!\right|_h^2+s_h\left(\mathcal{F}_{\Sigma_{\delta, \mathrm{D}}^{\pm}} ; \boldsymbol{u}, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right)+h^2 s_h\left(\mathcal{F}_{\Sigma_{\delta, \mathrm{N}}^{\pm}} ; \boldsymbol{u}, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right) \\
&\qquad +h^k C_k\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h \\
&\lesssim \left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}\right|\!\right|\!\right|_h^2+\tilde{s}_h\left(\mathcal{F}_{\Sigma_\delta^{\pm}} ; \boldsymbol{u}, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right)+h^k C_k\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h,
\end{aligned}
$$

where $C_k := \left[\|\boldsymbol{u}\|_{H^{\min\{k, 2\}+1}(\widehat{\mathfrak{D}})}+\|\boldsymbol{g}_{\mathrm{N}}\|_{H^{\min\{k, 2\}}(\widehat{\mathfrak{D}})}\right]$ comes from (4.38) and $\tilde{s}_h\left(\mathcal{F}_{\Sigma_\delta^{\pm}} ; \cdot, \cdot\right)$ includes the h^2 weighting on $\Sigma_{\delta, \mathrm{N}}^{\pm}$. Applying another weighted Young's inequality on the last term with a well-chosen weight, we get

$$
\begin{aligned}
\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h^2 &\lesssim \left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}\right|\!\right|\!\right|_h^2+\tilde{s}_h\left(\mathcal{F}_{\Sigma_\delta^{\pm}} ; \boldsymbol{u}, \pi_h \boldsymbol{u}-\boldsymbol{u}_h\right)+h^{2k} C_k^2 \\
&\lesssim h^{2k}\|\boldsymbol{u}\|_{H^{k+1}(\Omega)}^2+\left(\tilde{s}_h\left(\mathcal{F}_{\Sigma_\delta^{\pm}} ; \boldsymbol{u}, \boldsymbol{u}\right)\right)^{1/2}\left(\tilde{s}_h\left(\mathcal{F}_{\Sigma_\delta^{\pm}} ; \boldsymbol{v}_h, \boldsymbol{v}_h\right)\right)^{1/2}+h^{2k} C_k^2
\end{aligned}
$$

where, for brevity, we denote $\boldsymbol{v}_h := \pi_h \boldsymbol{u}-\boldsymbol{u}_h$, and we used Prop. 4.17. Again, we use a weighted Young's inequality to obtain

$$
\begin{aligned}
\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h^2 &\lesssim h^{2k}\left(\|\boldsymbol{u}\|_{H^{k+1}(\Omega)}^2+C_k^2\right)+\frac{\epsilon}{2} s_h\left(\mathcal{F}_{\Sigma_\delta^{\pm}} ; \boldsymbol{u}, \boldsymbol{u}\right)+\frac{1}{2 \epsilon} s_h\left(\mathcal{F}_{\Sigma_\delta^{\pm}} ; \boldsymbol{v}_h, \boldsymbol{v}_h\right) \\
&\lesssim h^{2k}\left(\left(1+\frac{\epsilon}{2}\right)\|\boldsymbol{u}\|_{H^{k+1}(\Omega)}^2+C_k^2\right)+\frac{1}{2 \epsilon}\left|\!\left|\!\left|\pi_h \boldsymbol{u}-\boldsymbol{u}_h\right|\!\right|\!\right|_h^2,
\end{aligned}
$$

where we used (4.11), the properties of the bounded extension operator, and the definition of $|||\cdot|||_h$. By choosing ϵ appropriately, we combine the far right term with the left-hand-side to get

$$|||\pi_h \boldsymbol{u} - \boldsymbol{u}_h|||_h^2 \lesssim h^{2k} \Big[\|\boldsymbol{u}\|_{H^{k+1}(\Omega)} + \|\boldsymbol{g}_{\mathrm{N}}\|_{H^{\min\{k,2\}}(\widehat{\mathfrak{D}})} \Big]^2.$$

Combining this result with (4.40) gives the first line of (4.39). The second line follows by a classic duality argument [37]. □

Chapter 5. Unfitted Shape Derivatives

We start with a review of basic shape differentiability results [22, 39] based on vector displacements of the domain. Next, we extend these shape derivatives to allow for perturbation of the domain by perturbing its level set description. Then, we develop these results further to allow for shape functionals over domains that intersect a fixed Lipschitz subset (i.e. an element of a finite element mesh).

5.1. Fréchet Differentiability of Shape Functionals

We review the Fréchet differentiability of shape functionals following [39, 1]. A classic approach to shape differentiation uses a perturbation of the identity. Let $\boldsymbol{U} \in [W^{1,\infty}(\mathbb{R}^d)]^d$ be a vector field and define the deformation mapping as follows

$$\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a}) := \mathbf{id}(\boldsymbol{a}) + \boldsymbol{U}(\boldsymbol{a}), \quad \text{for all } \boldsymbol{a} \in \mathbb{R}^d. \tag{5.1}$$

This mapping induces a deformed domain $\Omega_{\boldsymbol{U}} := \boldsymbol{\Phi}_{\boldsymbol{U}}(\Omega)$. For $\|\boldsymbol{U}\|_{W^{1,\infty}}$ sufficiently small, if Ω is Lipschitz, then $\Omega_{\boldsymbol{U}}$ will also be Lipschitz and homeomorphic to Ω [22]. We have the following definition [1, Defn. 4.1].

Definition 5.1. *Let Ω be Lipschitz. A shape functional $J(\Omega)$ is said to be* shape differentiable *at Ω if the mapping $\boldsymbol{U} \mapsto J(\Omega_{\boldsymbol{U}})$ from $[W^{1,\infty}(\mathbb{R}^d)]^d$ into $\mathbb{R}$, where $\Omega_{\boldsymbol{U}} = \boldsymbol{\Phi}_{\boldsymbol{U}}(\Omega)$ using* (5.1)*, is Fréchet differentiable at $\boldsymbol{U} = \mathbf{0}$. The Fréchet derivative of J at Ω is an operator in $\mathcal{L}([W^{1,\infty}(\mathbb{R}^d)]^d, \mathbb{R})$, denoted $J'(\Omega)(\cdot)$, and the following limit holds*

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0} \frac{|J(\Omega_{\boldsymbol{U}}) - J(\Omega) - J'(\Omega)(\boldsymbol{U})|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0. \tag{5.2}$$

We note a classic expansion of the determinant from [76, Lem. B.2].

Lemma 5.2. *For any $n \times n$ matrix B, such that $|B| < 1$, we have*

$$\det(I + B) = 1 + \operatorname{tr}(B) + \frac{1}{2}\left[(\operatorname{tr}(B))^2 - \operatorname{tr}\left(B^2\right)\right] + O(|B|^3), \tag{5.3}$$

The next two lemmas are applications of results in [22, 39]. We include the proofs of both Lemmas since we build on it later when computing shape derivatives on "cut" elements.

Lemma 5.3. *Given $f \in L^1(\mathbb{R}^d)$ and $\boldsymbol{U} \in [W^{1,\infty}(\mathbb{R}^d)]^d$ we have that*

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0} \frac{\int_\Omega [f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})]\, G(\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})) d\boldsymbol{a}}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0, \tag{5.4}$$

where $G : \mathbb{R}^{d\times d} \to \mathbb{R}$ is continuous and $|G(M)| \le C|M|$ for all $M \in \mathbb{R}^{d\times d}$, for some bounded constant $C > 0$.

Proof. We have that

$$\begin{aligned} I_0(\boldsymbol{U}) &:= \frac{|\int_\Omega [f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})]\, G(\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})) d\boldsymbol{a}|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} \\ &\le C \int_\Omega |f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})| d\boldsymbol{a} \frac{\|\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})\|_\infty}{\|\boldsymbol{U}\|_{W^{1,\infty}}} \le C \int_\Omega |f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})| d\boldsymbol{a}. \end{aligned}$$

Next, let $\{f_k\}$ be a sequence in $C^\infty(\mathbb{R}^d)$ such that $f_k \to f$ in L^1 as $k \to \infty$. Then, for any $k \ge 1$, we have

$$\begin{aligned} I_0(\boldsymbol{U}) &\lesssim \int_\Omega |(f - f_k)(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - (f - f_k)(\boldsymbol{a})| d\boldsymbol{a} + \int_\Omega |f_k(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f_k(\boldsymbol{a})| d\boldsymbol{a} \\ &\le \int_\Omega |(f - f_k)(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a}))| d\boldsymbol{a} + \|f - f_k\|_{L^1(\mathbb{R}^d)} + \int_\Omega |f_k(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f_k(\boldsymbol{a})| d\boldsymbol{a} \\ &= \int_{\boldsymbol{\Phi}_{\boldsymbol{U}}^{-1}(\Omega)} |(f - f_k)(\boldsymbol{x})| \det(\nabla \boldsymbol{\Phi}_{\boldsymbol{U}}^{-1}) d\boldsymbol{x} + \|f - f_k\|_{L^1(\mathbb{R}^d)} + \int_\Omega |f_k(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f_k(\boldsymbol{a})| d\boldsymbol{a} \\ &\le (C_{\boldsymbol{U}} + 1)\|f - f_k\|_{L^1(\mathbb{R}^d)} + \int_\Omega \int_0^1 |\nabla f_k(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))||\boldsymbol{U}(\boldsymbol{a})| ds d\boldsymbol{a}, \end{aligned}$$

where $C_{\boldsymbol{U}} > 0$ is a bounded constant for all $\boldsymbol{U}$ such that $\|\boldsymbol{U}\|_{W^{1,\infty}}$ is sufficiently small, and we used the fundamental theorem of calculus for line integrals:

$$f_k(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f_k(\boldsymbol{a}) = \int_0^1 \nabla f_k(\boldsymbol{a} + s\boldsymbol{U}(\boldsymbol{a})) \cdot \boldsymbol{U}(\boldsymbol{a}) ds.$$

Letting $C_k := \max_{\boldsymbol{a}\in\Omega, 0\leq s\leq 1} |\nabla f_k(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))|$, we get

$$I_0(\boldsymbol{U}) \leq C(C_{\boldsymbol{U}} + 1)\|f - f_k\|_{L^1(\mathbb{R}^d)} + CC_k|\Omega| \cdot \|\boldsymbol{U}\|_{L^\infty}$$

Hence,

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0} I_0(\boldsymbol{U}) \leq C(C_{\boldsymbol{U}} + 1)\|f - f_k\|_{L^1(\mathbb{R}^d)},$$

for all $k \geq 1$. Since the left-side is independent of k, we have that $\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0} I_0(\boldsymbol{U}) = 0$, thus proving the assertion. □

Lemma 5.4. *Given $f \in W^{1,1}(\mathbb{R}^d)$ and $\boldsymbol{U} \in [W^{1,\infty}(\mathbb{R}^d)]^d$ we have that*

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0} \frac{\int_\Omega f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})d\boldsymbol{a} - \int_\Omega \nabla f(\boldsymbol{a}) \cdot \boldsymbol{U}(\boldsymbol{a})d\boldsymbol{a}}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0. \tag{5.5}$$

Proof. By the fundamental theorem of calculus, we have

$$f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a}) = \int_0^1 \nabla f(\boldsymbol{a} + s\boldsymbol{U}(\boldsymbol{a})) \cdot \boldsymbol{U}(\boldsymbol{a})ds, \tag{5.6}$$

and so

$$\begin{aligned} I_0(\boldsymbol{U}) &:= \int_\Omega f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})d\boldsymbol{a} - \int_\Omega \nabla f(\boldsymbol{a}) \cdot \boldsymbol{U}(\boldsymbol{a})d\boldsymbol{a} \\ &= \int_\Omega \int_0^1 \nabla f(\boldsymbol{a} + s\boldsymbol{U}(\boldsymbol{a})) \cdot \boldsymbol{U}(\boldsymbol{a})dsd\boldsymbol{a} - \int_\Omega \nabla f(\boldsymbol{a}) \cdot \boldsymbol{U}(\boldsymbol{a})d\boldsymbol{a} \\ &= \int_\Omega \int_0^1 [\nabla f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f(\boldsymbol{a})] \cdot \boldsymbol{U}(\boldsymbol{a})dsd\boldsymbol{a}, \end{aligned} \tag{5.7}$$

and note that by Prop. 4.12, $\nabla f \circ \boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})$ can be viewed as function in $L^1(\mathbb{R}^d \times [0,1])$, provided $\|\boldsymbol{U}\|_{W^{1,\infty}}$ is sufficiently small. Indeed, the entire integrand in the last integral of

(5.7) is in $L^1(\mathbb{R}^d \times [0,1])$. Therefore, we can apply Fubini's theorem:

$$
\begin{aligned}
\frac{|I_0(\boldsymbol{U})|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} &= \frac{1}{\|\boldsymbol{U}\|_{W^{1,\infty}}} \left| \int_0^1 \int_\Omega [\nabla f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f(\boldsymbol{a})] \cdot \boldsymbol{U}(\boldsymbol{a}) d\boldsymbol{a} ds \right| \\
&\leq \int_0^1 \int_\Omega |\nabla f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f(\boldsymbol{a})| \, d\boldsymbol{a} ds \\
&\leq \int_0^1 \int_\Omega |\nabla (f - f_k)(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))| \, d\boldsymbol{a} ds + \int_0^1 \int_\Omega |\nabla (f - f_k)(\boldsymbol{a})| \, d\boldsymbol{a} ds \\
&\quad + \int_0^1 \int_\Omega |\nabla f_k(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f_k(\boldsymbol{a})| \, d\boldsymbol{a} ds,
\end{aligned}
\tag{5.8}
$$

where we introduced a sequence $\{f_k\}$ in $C^\infty(\mathbb{R}^d)$ such that $f_k \to f$ in $W^{1,1}$ as $k \to \infty$. We apply a change of variables to the first term:

$$
\begin{aligned}
\int_0^1 \int_\Omega |\nabla (f - f_k)(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))| \, d\boldsymbol{a} ds &= \int_0^1 \int_{\boldsymbol{\Phi}_{s\boldsymbol{U}}^{-1}(\Omega)} |\nabla (f - f_k)(\boldsymbol{x})| \det(\nabla \boldsymbol{\Phi}_{s\boldsymbol{U}}^{-1}(\boldsymbol{x})) d\boldsymbol{x} ds \\
&\leq \gamma_0 \|f - f_k\|_{W^{1,1}(\mathbb{R}^d)},
\end{aligned}
$$

where γ_0 is a bounded constant when $\|\boldsymbol{U}\|_{W^{1,\infty}(\mathbb{R}^d)}$ is sufficiently small. The last term in (5.8) is estimated with the mean value theorem to give

$$
\int_0^1 \int_\Omega |\nabla f_k(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f_k(\boldsymbol{a})| \, d\boldsymbol{a} ds \leq C_k \|\boldsymbol{U}\|_{L^\infty(\mathbb{R}^d)},
$$

where C_k depends on $\|\nabla\nabla f_k\|_{L^\infty}$. Thus,

$$
\begin{aligned}
\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0} \frac{|I_0(\boldsymbol{U})|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} &\leq \lim_{\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0} (\gamma_0 + 1) \|f - f_k\|_{W^{1,1}(\mathbb{R}^d)} + C_k \|\boldsymbol{U}\|_{L^\infty(\mathbb{R}^d)} \\
&\leq (\gamma_0 + 1) \|f - f_k\|_{W^{1,1}(\mathbb{R}^d)}
\end{aligned}
$$

which holds for every $k \geq 1$. Taking $k \to \infty$ proves (5.5). □

The following result is an application of the results in [22, 39, 1].

Theorem 5.5. *For the shape functional $J(\Omega) := \int_\Omega f(\boldsymbol{x}) d\boldsymbol{x}$ with $f \in W^{1,1}(\mathbb{R}^d)$ we have that $J(\Omega)$ is shape differentiable at Ω (in the sense of Definition 5.1) with Fréchet derivative $J'(\Omega)(\boldsymbol{U}) = \int_{\partial\Omega} f(\boldsymbol{a}) \boldsymbol{U}(\boldsymbol{a}) \cdot \boldsymbol{\nu}(\boldsymbol{a}) d\boldsymbol{a}$ for all $\boldsymbol{U} \in [W^{1,\infty}(\mathbb{R}^d)]^d$.*

Proof. Using (5.3), we begin with

$$
\begin{aligned}
J(\Omega_{\boldsymbol{U}}) - J(\Omega) &= \int_{\Omega_{\boldsymbol{U}}} f(\boldsymbol{x}) d\boldsymbol{x} - \int_{\Omega} f(\boldsymbol{a}) d\boldsymbol{a} \\
&= \int_{\Omega} f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) \det(I + \nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})) d\boldsymbol{a} - \int_{\Omega} f(\boldsymbol{a}) d\boldsymbol{a} \\
&= \int_{\Omega} f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a}) d\boldsymbol{a} + \int_{\Omega} f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) \mathrm{tr}(\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})) d\boldsymbol{a} \\
&\quad + \int_{\Omega} f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) O(|\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})|^2) d\boldsymbol{a} \\
&= \int_{\Omega} f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a}) d\boldsymbol{a} + \int_{\Omega} \nabla_{\boldsymbol{a}} \cdot [f(\boldsymbol{a}) \boldsymbol{U}(\boldsymbol{a})] d\boldsymbol{a} - \int_{\Omega} \nabla_{\boldsymbol{a}} f(\boldsymbol{a}) \cdot \boldsymbol{U}(\boldsymbol{a}) d\boldsymbol{a} \\
&\quad + \int_{\Omega} [f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})] \nabla_{\boldsymbol{a}} \cdot \boldsymbol{U}(\boldsymbol{a}) d\boldsymbol{a} + \int_{\Omega} f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) O(|\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})|^2) d\boldsymbol{a}.
\end{aligned}
$$

By Gauss' divergence theorem, we have

$$
\begin{aligned}
J'(\Omega)(\boldsymbol{U}) &= \int_{\partial\Omega} f(\boldsymbol{a}) \boldsymbol{U}(\boldsymbol{a}) \cdot \boldsymbol{\nu}(\boldsymbol{a}) d\boldsymbol{a} \\
&= \int_{\Omega} \nabla_{\boldsymbol{a}} \cdot [f(\boldsymbol{a}) \boldsymbol{U}(\boldsymbol{a})] d\boldsymbol{a}
\end{aligned}
$$

So then, by Lemmas 5.3, 5.4, we find that

$$
\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0} \frac{J(\Omega_{\boldsymbol{U}}) - J(\Omega) - J'(\Omega)(\boldsymbol{U})}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0,
$$

meaning that $J(\Omega)$ is Fréchet differentiable with $J'(\Omega)(\boldsymbol{U}) = \int_{\partial\Omega} f(\boldsymbol{a}) \boldsymbol{U}(\boldsymbol{a}) \cdot \boldsymbol{\nu}(\boldsymbol{a}) d\boldsymbol{a}$ being the Fréchet derivative. Note that, by Sobolev embedding, $f \in W^{1,1}(\Omega)$ implies $f \in L^1(\partial\Omega)$. □

5.2. Connecting the Domain Perturbation with the Level Set Perturbation

Our goal is to obtain a shape differentiation formula in terms of perturbations of the level set representation ϕ of Ω (see Section 3.1), since this is more convenient for the optimization algorithm. See also [58, 47].

5.2.1. The Speed Method

We first review the velocity (speed) method for domain perturbations. Let $\boldsymbol{V}(\boldsymbol{x}, t)$ be a d-dimensional, vector field that is Lipschitz in $\boldsymbol{x}$, for each t, and continuously differentiable in t for each $\boldsymbol{x}$. For any given $\boldsymbol{a} \in \mathbb{R}^d$, consider the following ODE:

$$\dot{\boldsymbol{x}} = \boldsymbol{V}(\boldsymbol{x}, t),\ \forall\, t > 0, \qquad \boldsymbol{x}(0) = \boldsymbol{a} \in \mathbb{R}^d, \tag{5.9}$$

with unique solution (see [35]) $\boldsymbol{x}(t)$ being the trajectory of a (material) point $\boldsymbol{a}$ moving with velocity $\boldsymbol{V}(\boldsymbol{x}(t), t)$. Indeed, $\boldsymbol{V}$ induces a deformation mapping through (5.9) in the following way. Let $\boldsymbol{x}(t; \boldsymbol{a})$ be the unique solution of (5.9) (for a given $\boldsymbol{a}$). Then,

$$\boldsymbol{\Phi}_t(\boldsymbol{a}) := \boldsymbol{x}(t; \boldsymbol{a}), \quad \text{for all } \boldsymbol{a} \in \mathbb{R}^d, \tag{5.10}$$

is the corresponding deformation mapping. Moreover, a Taylor expansion in t yields

$$\boldsymbol{\Phi}_t(\boldsymbol{a}) = \boldsymbol{a} + t\boldsymbol{V}(\boldsymbol{a}, 0) + \boldsymbol{W}(\boldsymbol{a}, t), \quad \text{for all } \boldsymbol{a} \in \mathbb{R}^d, \tag{5.11}$$

where $|\boldsymbol{W}(\boldsymbol{a}, t)| = O(t^2)$. With this, one can establish the Gâteaux shape differentiablity of our shape functional $J(\Omega) = \int_\Omega f(\boldsymbol{x})\, d\boldsymbol{x}$, for $f \in W^{1,1}(\mathbb{R}^d)$, with respect to $\boldsymbol{V}(\boldsymbol{x}(0), 0)$ using classic techniques. In other words, setting $\Omega_t = \boldsymbol{\Phi}_t(\Omega)$, we have

$$d_G J(\Omega)(\boldsymbol{V}) := \lim_{t \to 0^+} \frac{J(\Omega_t) - J(\Omega)}{t} = \int_{\partial\Omega} f(\boldsymbol{a}) \boldsymbol{V}(\boldsymbol{a}, 0) \cdot \boldsymbol{\nu}(\boldsymbol{a}) d\boldsymbol{a}, \tag{5.12}$$

which, of course, agrees with the result in Theorem 5.5 if $\boldsymbol{U}(\boldsymbol{a}) \equiv \boldsymbol{V}(\boldsymbol{a}, 0)$. The same result holds if the remainder term in (5.11) is dropped.

5.2.2. Level Set Gâteaux Derivative

Now, we consider Ω to be defined by a level set function, ϕ, i.e. $\Omega(\phi) := \{\boldsymbol{x} \in \mathbb{R}^d : \phi(\boldsymbol{x}) < 0\}$ (sub-zero level set), where ϕ satisfies Definition 5.6 for some positive constants c_0 and δ_0.

Definition 5.6. *Let* $\phi \in C^{0,1}(\mathbb{R}^d; \mathbb{R})$ *and assume that* $\Gamma(\phi) := \{\boldsymbol{x} \in \mathbb{R}^d : \phi(\boldsymbol{x}) = 0\}$ *is non-empty. We say that* ϕ *is* non-degenerate, with constants $c_0 > 0$ and $\delta_0 > 0$, *if* $|\nabla\phi(\boldsymbol{x})| \geq c_0$ *for a.e.* $\boldsymbol{x} \in \mathbb{R}^d$ *such that* $\operatorname{dist}(\boldsymbol{x}, \Gamma(\phi)) < \delta_0$.

In addition, we take ϕ to be $C^2(\mathbb{R}^d)$. By [22, Ch. 2, Thm. 4.2], $\Omega(\phi)$ is a C^2, open set, and $\partial\Omega(\phi) \equiv \Gamma(\phi)$, so $\Omega(\phi)$ is well-defined. For the shape functional, $J(\Omega)$, we seek to compute the Gâteaux shape derivative with respect to ϕ, i.e.

$$d_G J(\Omega(\phi))(\eta) := \lim_{t \to 0^+} \frac{J(\Omega(\phi + t\eta)) - J(\Omega(\phi))}{t}, \tag{5.13}$$

for any $\eta \in C^2(\mathbb{R}^d)$. We will derive an explicit formula for (5.13) using (5.12). Define a perturbed level set function

$$\tilde{\phi}(\boldsymbol{x}, t) = \phi(\boldsymbol{x}) + t\eta(\boldsymbol{x}), \quad \Rightarrow \quad \partial_t \tilde{\phi} = \eta, \tag{5.14}$$

where t is the perturbation parameter; one can think of $\tilde{\phi}$ as a time-dependent level set function. Set $\Omega_t := \Omega(\tilde{\phi}(\cdot, t)) = \{\boldsymbol{x} \in \mathbb{R}^d : \tilde{\phi}(\boldsymbol{x}, t) < 0\}$ and $\Gamma_t := \partial\Omega_t = \{\boldsymbol{x} \in \mathbb{R}^d : \tilde{\phi}(\boldsymbol{x}, t) = 0\}$. Note that $|\nabla\tilde{\phi}(\boldsymbol{x}, t)| \geq c_0/2 > 0$ for all $\boldsymbol{x}$ in a neighborhood of Γ_t if t is sufficiently small. This ensures that Γ_t is (locally) a C^2 surface by the implicit function theorem. Next, define a velocity field

$$\boldsymbol{V}(\boldsymbol{x}, t) = -\frac{\nabla\tilde{\phi}(\boldsymbol{x}, t)}{|\nabla\tilde{\phi}(\boldsymbol{x}, t)|^2}\eta(\boldsymbol{x}), \tag{5.15}$$

which satisfies the same conditions for $\boldsymbol{V}$ in (5.9), and let $\boldsymbol{x}(t)$ be the corresponding solution of (5.9). If $\boldsymbol{x}(0) = \boldsymbol{a} \in \Gamma_0$, we have that $\tilde{\phi}(\boldsymbol{x}(t), t) = 0$ for all t because

$$\begin{aligned}\frac{d}{dt}\tilde{\phi}(\boldsymbol{x}(t), t) \equiv D_{\boldsymbol{V}}\tilde{\phi}(\boldsymbol{x}, t)\Big|_{\boldsymbol{x}=\boldsymbol{x}(t)} &= \partial_t\tilde{\phi}(\boldsymbol{x}, t)\Big|_{\boldsymbol{x}=\boldsymbol{x}(t)} + \left(\nabla\tilde{\phi}(\boldsymbol{x}, t)\Big|_{\boldsymbol{x}=\boldsymbol{x}(t)}\right) \cdot \dot{\boldsymbol{x}}(t) \\ &= \eta(\boldsymbol{x}(t)) + \nabla\tilde{\phi}(\boldsymbol{x}(t), t) \cdot \boldsymbol{V}(\boldsymbol{x}(t), t) = 0.\end{aligned}$$

Thus, $\boldsymbol{V}$ evolves the zero level set of $\tilde{\phi}$. Moreover, if $\boldsymbol{\Phi}_t(\boldsymbol{a})$ is the induced map from $\boldsymbol{V}$, then the sub-zero level set Ω_t satisfies $\Omega_t = \boldsymbol{\Phi}_t(\Omega_0)$. With this, one can compute (5.13) by using (5.12), i.e.

$$\begin{aligned}
d_G J(\Omega(\phi))(\eta) &= \lim_{t \to 0^+} \frac{J(\Omega(\phi + t\eta)) - J(\Omega(\phi))}{t} \\
&= \lim_{t \to 0^+} \frac{J(\Omega_t) - J(\Omega_0)}{t} \\
&= \int_{\partial\Omega} f(\boldsymbol{a}) \boldsymbol{V}(\boldsymbol{a}, 0) \cdot \boldsymbol{\nu}(\boldsymbol{a}) d\boldsymbol{a} \\
&= \int_{\partial\Omega} f(\boldsymbol{a}) \left(-\frac{\nabla \tilde{\phi}(\boldsymbol{a}, 0)}{|\nabla \tilde{\phi}(\boldsymbol{a}, 0)|^2} \eta(\boldsymbol{a}) \right) \cdot \boldsymbol{\nu}(\boldsymbol{a}) d\boldsymbol{a} \\
&= \int_{\partial\Omega} f(\boldsymbol{a}) \left(-\frac{\eta(\boldsymbol{a})}{|\nabla \phi(\boldsymbol{a})|} \right) d\boldsymbol{a},
\end{aligned}$$

where we used the fact that $\boldsymbol{\nu} = \nabla\phi / |\nabla\phi|$ on $\partial\Omega$ and $\tilde{\phi}(\boldsymbol{a}, 0) = \phi(\boldsymbol{a})$. All of the above extends to having ϕ, η in $W^{2,\infty}(\mathbb{R}^d)$; in this case, $\Omega(\phi)$ is a $C^{1,1}$ domain [22, Ch. 5, Thm 4.3].

5.2.3. Level Set Fréchet Derivative

Our goal now is to extend this to computing the Fréchet shape derivative of $J(\Omega(\phi))$ with respect to ϕ, which is defined as follows.

Definition 5.7. *Let $\Omega = \Omega(\phi)$ be the sub-zero level set of $\phi \in \mathcal{X}$ that satisfies Definition 5.6 for some positive constants c_0 and δ_0. A shape functional $J(\phi) \equiv J(\Omega(\phi))$ is said to be* level set shape Fréchet differentiable *at ϕ if the mapping $\eta \mapsto J(\Omega(\phi + \eta))$ from $\mathcal{X}$ into $\mathbb{R}$ is Fréchet differentiable at $\eta = 0$. The Fréchet derivative of $J(\Omega(\cdot))$, at ϕ, is an operator in $\mathcal{L}(\mathcal{X}, \mathbb{R})$, denoted $J'(\Omega(\phi))(\cdot)$, and the following limit holds*

$$\lim_{\|\eta\|_{\mathcal{X}} \to 0} \frac{|J(\Omega(\phi + \eta)) - J(\Omega(\phi)) - J'(\Omega(\phi))(\eta)|}{\|\eta\|_{\mathcal{X}}} = 0. \tag{5.16}$$

In this section, we use Definition 5.7 with $\mathcal{X} = W^{2,\infty}(\mathbb{R}^d)$. Moreover, we shall prove that $J(\Omega) = \int_\Omega f(\boldsymbol{x})\, d\boldsymbol{x}$ is level set shape Fréchet differentiable by using Theorem 5.5. To do this, we have to reconcile two different, but similar, notions of domain perturbation.

The first is the perturbed domain $\Omega(\phi + \eta)$ and the second is through a perturbation of the identity approach given by

$$\boldsymbol{\Phi}_\eta(\boldsymbol{a}) = \boldsymbol{a} + \boldsymbol{V}_\eta(\boldsymbol{a}), \quad \text{for all } \boldsymbol{a} \in \mathbb{R}^d, \quad \boldsymbol{V}_\eta(\boldsymbol{a}) := -\frac{\nabla\phi(\boldsymbol{a})}{|\nabla\phi(\boldsymbol{a})|^2}\eta(\boldsymbol{a}). \tag{5.17}$$

Note the similarity with $\boldsymbol{\Phi}_t$ from (5.11) and (5.15), but $\boldsymbol{\Phi}_t$ is not the same as $\boldsymbol{\Phi}_\eta$. Recall $\boldsymbol{\Phi}_t$ satisfies (5.9) with $\boldsymbol{V}$ given by (5.15), and note that $\nabla_{\boldsymbol{a}}\boldsymbol{\Phi}_t(\boldsymbol{a})$ uniquely satisfies the matrix valued ODE [22, Ch. 8]:

$$\frac{d}{dt}M(\boldsymbol{a}, t) = [\nabla_{\boldsymbol{x}}\boldsymbol{V}(\boldsymbol{\Phi}_t(\boldsymbol{a}), t)]M(\boldsymbol{a}, t), \ \forall\, t > 0, \quad M(\boldsymbol{a}, 0) = I, \quad \forall\, \boldsymbol{a} \in \mathbb{R}^d, \tag{5.18}$$

which follows by the theory in [35]. Furthermore, we have an explicit formula for $\nabla_{\boldsymbol{a}}\boldsymbol{\Phi}_t(\boldsymbol{a})$:

$$\nabla_{\boldsymbol{a}}\boldsymbol{\Phi}_t(\boldsymbol{a}) = \exp\left\{\int_0^t \nabla_{\boldsymbol{x}}\boldsymbol{V}(\boldsymbol{x}(s;\boldsymbol{a}), s)\, ds\right\} =: A(t), \tag{5.19}$$

where $\exp\{\cdot\}$ is the matrix exponential.

Theorem 5.8. *Let $\{\phi_k\}_{k\geq 1}$ be a sequence of smooth functions such that $\|\phi_k - \phi\|_{W^{2,\infty}} \to 0$ as $k \to \infty$. Assume $|\nabla\phi| \geq c_0 > 0$ and $|\nabla\eta| \leq c_0/2$, so that $|\nabla(\phi+\eta)| \geq c_0/2$. In addition, assume $\|\eta\|_{W^{2,\infty}} \leq c_1$ for some fixed constant c_1. Set $\widetilde{\boldsymbol{\Phi}} = \boldsymbol{\Phi}_t|_{t=1}$. Then,*

$$\begin{aligned} \|\boldsymbol{\Phi}_\eta - \widetilde{\boldsymbol{\Phi}}\|_{L^\infty(\mathbb{R}^d)} &\leq O\left(\|\eta\|_{L^\infty}\|\eta\|_{W^{1,\infty}}\right), \\ \|\nabla\boldsymbol{\Phi}_\eta - \nabla\widetilde{\boldsymbol{\Phi}}\|_{L^\infty(\mathbb{R}^d)} &\leq O\left(\|\eta\|^2_{W^{2,\infty}}\right) + q_1\|\phi_k\|_{W^{3,\infty}}\|\eta\|^2_{L^\infty} + q_2\|\phi_k - \phi\|_{W^{2,\infty}}\|\eta\|_{L^\infty}, \end{aligned} \tag{5.20}$$

for all $k \geq 1$, for some bounded constants q_1, q_2.

Proof. Recall that $\boldsymbol{\Phi}_t$ is defined in Section 5.2.1 and is different from $\boldsymbol{\Phi}_\eta$. For now, take

$\boldsymbol{a} \in \mathbb{R}^d$ fixed and note that the solution of (5.9) satisfies:

$$
\begin{aligned}
|\boldsymbol{x}(t) - \boldsymbol{a}| &= \left| \int_0^t \boldsymbol{V}(\boldsymbol{x}(s), s)\, ds \right| \\
&= \left| \int_0^t \frac{\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))}{|\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))|^2} \eta(\boldsymbol{x}(s))\, ds \right| \\
&\leq \left| \int_0^t \frac{\eta(\boldsymbol{x}(s))}{|\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))|}\, ds \right| \\
&\leq \frac{2}{c_0} \|\eta\|_{L^\infty},\ 0 \leq t \leq 1,
\end{aligned}
\tag{5.21}
$$

for some constant C depending on c_0. We first estimate $\|\boldsymbol{\Phi}_\eta - \widetilde{\boldsymbol{\Phi}}\|_{L^\infty(\mathbb{R}^d)}$ and we start with

$$
\begin{aligned}
\boldsymbol{V}_\eta(\boldsymbol{a}) - \boldsymbol{V}(\boldsymbol{x}(s), s) &= \frac{\nabla\phi(\boldsymbol{a})}{|\nabla\phi(\boldsymbol{a})|^2}\eta(\boldsymbol{a}) - \frac{\nabla[\phi(\boldsymbol{x}(s)) + s\eta(\boldsymbol{x}(s))]}{|\nabla[\phi(\boldsymbol{x}(s)) + s\eta(\boldsymbol{x}(s))]|^2}\eta(\boldsymbol{x}(s)) \\
&= T_1 + T_2 + T_3,
\end{aligned}
\tag{5.22}
$$

where

$$
\begin{aligned}
T_1 &= \frac{1}{|\nabla\phi(\boldsymbol{a})|^2} \left(\eta(\boldsymbol{a})\nabla\phi(\boldsymbol{a}) - \eta(\boldsymbol{x}(s))\nabla\phi(\boldsymbol{x}(s)) \right), \\
T_2 &= -\frac{s}{|\nabla\phi(\boldsymbol{a})|^2}\eta(\boldsymbol{x}(s))\nabla\eta(\boldsymbol{x}(s)), \\
T_3 &= \eta(\boldsymbol{x}(s))\nabla[\phi(\boldsymbol{x}(s)) + s\eta(\boldsymbol{x}(s))] \left(\frac{|\nabla[\phi(\boldsymbol{x}(s)) + s\eta(\boldsymbol{x}(s))]|^2 - |\nabla\phi(\boldsymbol{a})|^2}{|\nabla\phi(\boldsymbol{a})|^2 |\nabla[\phi(\boldsymbol{x}(s)) + s\eta(\boldsymbol{x}(s))]|^2} \right).
\end{aligned}
\tag{5.23}
$$

Next, we note the following basic estimates:

$$
|\nabla\phi(\boldsymbol{x}(s)) - \nabla\phi(\boldsymbol{a})| = |\nabla^2\phi(\boldsymbol{x}(\xi)) \cdot (\boldsymbol{x}(s) - \boldsymbol{a})| \leq C\|\nabla^2\phi\|_{L^\infty}\|\eta\|_{L^\infty},
$$

$$
|\eta(\boldsymbol{x}(s)) - \eta(\boldsymbol{a})| = |\nabla\eta(\boldsymbol{x}(\xi)) \cdot (\boldsymbol{x}(s) - \boldsymbol{a})| \leq C\|\nabla\eta\|_{L^\infty}\|\eta\|_{L^\infty},
$$

for some bounded constant C. Using these estimates, we obtain the following:

$$\begin{aligned}
|T_1| &= \frac{1}{|\nabla\phi(\boldsymbol{a})|^2}\,|\eta(\boldsymbol{a})\nabla\phi(\boldsymbol{a}) - \eta(\boldsymbol{x}(s))\nabla\phi(\boldsymbol{x}(s))| \\
&\le \frac{1}{|\nabla\phi(\boldsymbol{a})|^2}\Big[\,|\eta(\boldsymbol{a})\nabla\phi(\boldsymbol{a}) - \eta(\boldsymbol{a})\nabla\phi(\boldsymbol{x}(s))| + |\eta(\boldsymbol{a})\nabla\phi(\boldsymbol{x}(s)) - \eta(\boldsymbol{x}(s))\nabla\phi(\boldsymbol{x}(s))|\,\Big] \\
&\lesssim \|\eta\|_{L^\infty}^2 + \|\nabla\eta\|_{L^\infty}\|\eta\|_{L^\infty} \\
|T_2| &= \frac{|s|}{|\nabla\phi(\boldsymbol{a})|^2}|\eta(\boldsymbol{x}(s))\nabla\eta(\boldsymbol{x}(s))| \\
&\lesssim \|\nabla\eta\|_{L^\infty}\|\eta\|_{L^\infty} \\
|T_3| &= |\eta(\boldsymbol{x}(s))\nabla[\phi(\boldsymbol{x}(s)) + s\eta(\boldsymbol{x}(s))]| \cdot \left|\frac{|\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))|^2 - |\nabla\phi(\boldsymbol{a})|^2}{|\nabla\phi(\boldsymbol{a})|^2|\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))|^2}\right| \\
&\le \|\eta\|_{L^\infty} \cdot \frac{\Big||\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))| - |\nabla\phi(\boldsymbol{a})|\Big| \cdot \Big[|\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))| + |\nabla\phi(\boldsymbol{a})|\Big]}{|\nabla\phi(\boldsymbol{a})|^2|\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))|} \\
&\lesssim \|\eta\|_{L^\infty} \cdot \Big||\nabla\phi(\boldsymbol{x}(s)) + s\nabla\eta(\boldsymbol{x}(s))| - |\nabla\phi(\boldsymbol{a})|\Big| \\
&\le \|\nabla\eta\|_{L^\infty}\|\eta\|_{L^\infty}
\end{aligned}$$

Hence, we have that

$$|T_1|, |T_2|, |T_3| \le C\|\eta\|_{L^\infty}\|\eta\|_{W^{1,\infty}}, \tag{5.24}$$

which gives a bound for (5.22). Since $\boldsymbol{x}(1) \equiv \tilde{\boldsymbol{\Phi}}(\boldsymbol{a}) = \boldsymbol{a} + \int_0^1 \boldsymbol{V}(\boldsymbol{x}(s), s)ds$, and $\boldsymbol{a}$ was arbitrary, we get

$$\|\boldsymbol{\Phi}_\eta - \tilde{\boldsymbol{\Phi}}\|_{L^\infty(\mathbb{R}^d)} = \left\|\int_0^1 \boldsymbol{V}_\eta(\boldsymbol{a}) - \boldsymbol{V}(\boldsymbol{x}(s), s)\, ds\right\| \le C\|\eta\|_{L^\infty}\|\eta\|_{W^{1,\infty}}. \tag{5.25}$$

Next, using that $\boldsymbol{V}_\eta(\boldsymbol{a}) \equiv \boldsymbol{V}(\boldsymbol{a}, 0)$, we estimate

$$\begin{aligned}
&\nabla\boldsymbol{V}(\boldsymbol{x}(s), s)A(s) - \nabla\boldsymbol{V}(\boldsymbol{a}, 0) = T_4 + T_5 \\
&\qquad\qquad T_4 := [\nabla\boldsymbol{V}(\boldsymbol{x}(s), s) - \nabla\boldsymbol{V}_\eta(\boldsymbol{a})]\,A(s), \\
&\qquad\qquad T_5 := \nabla\boldsymbol{V}_\eta(\boldsymbol{a})\,[A(s) - I]\,.
\end{aligned} \tag{5.26}$$

Estimating T_4 is similar to estimating (5.23). We first note that $|\nabla\eta(\boldsymbol{x}(s)) - \nabla\eta(\boldsymbol{a})| \leq C\|\nabla^2\eta\|_{L^\infty}\|\eta\|_{L^\infty}$, for some bounded constant C. Furthermore,

$$\begin{aligned}|\nabla^2\phi(\boldsymbol{x}(s)) - \nabla^2\phi(\boldsymbol{a})| &\leq |\nabla^2(\phi-\phi_k)(\boldsymbol{x}(s)) - \nabla^2(\phi-\phi_k)(\boldsymbol{a})| + |\nabla^2\phi_k(\boldsymbol{x}(s)) - \nabla^2\phi_k(\boldsymbol{a})| \\ &\leq 2\|\phi-\phi_k\|_{W^{2,\infty}} + |\nabla^3\phi_k(\boldsymbol{x}(\xi))\cdot(\boldsymbol{x}(s)-\boldsymbol{a})| \\ &\leq 2\|\phi-\phi_k\|_{W^{2,\infty}} + C\|\nabla^3\phi_k\|_{L^\infty}\|\eta\|_{L^\infty},\end{aligned} \tag{5.27}$$

for every $k \geq 1$. Next, by the properties of the matrix exponential, we have

$$|A(s) - I| \leq \int_0^s |\nabla_{\boldsymbol{x}}\boldsymbol{V}(\boldsymbol{x}(\mu;\boldsymbol{a}),\mu)|\, d\mu|A|(s), \quad |A|(s) = \exp\left\{\int_0^s |\nabla_{\boldsymbol{x}}\boldsymbol{V}(\boldsymbol{x}(\mu;\boldsymbol{a}),\mu)|\, d\mu\right\}. \tag{5.28}$$

Note that $|A(s)|$ is uniformly bounded for all $0 \leq s \leq 1$, and $|\nabla_{\boldsymbol{x}}\boldsymbol{V}(\boldsymbol{x}(\mu;\boldsymbol{a}),\mu)| \leq C\|\eta\|_{W^{1,\infty}}$ for sufficiently small η. Combining these estimates, and the usual arguments, we have

$$|\nabla\boldsymbol{V}(\boldsymbol{x}(s),s)A(s) - \nabla\boldsymbol{V}(\boldsymbol{a},0)| \leq C\left(\|\eta\|^2_{W^{2,\infty}} + \|\phi-\phi_k\|_{W^{2,\infty}}\|\eta\|_{L^\infty} + \|\nabla^3\phi_k\|_{L^\infty}\|\eta\|^2_{L^\infty}\right), \tag{5.29}$$

for all $0 \leq s \leq 1$. From this, we obtain the bound on $\|\nabla\boldsymbol{\Phi}_\eta - \nabla\widetilde{\boldsymbol{\Phi}}\|_{L^\infty}$ given in (5.20). □

Corollary 5.9. *Assume the hypothesis of Thm. 5.8 holds. Then,*

$$\|\det(\nabla\boldsymbol{\Phi}_\eta) - \det(\nabla\widetilde{\boldsymbol{\Phi}})\|_{L^\infty(\mathbb{R}^d)} \leq O\left(\|\eta\|^2_{W^{2,\infty}}\right) + q_1\|\phi_k\|_{W^{3,\infty}}\|\eta\|^2_{L^\infty} + q_2\|\phi_k - \phi\|_{W^{2,\infty}}\|\eta\|_{L^\infty}, \tag{5.30}$$

for all $k \geq 1$, for some bounded constants q_1, q_2.

Theorem 5.10. *Assume $\phi \in W^{2,\infty}(\mathbb{R}^d)$ and that it satisfies Definition 5.6 for some positive constants c_0, δ_0. Let $\Omega(\phi+\eta)$ be the sub-zero level set of $\phi+\eta$. For the shape func-*

tional $J(\Omega) := \int_\Omega f(\boldsymbol{x})d\boldsymbol{x}$ *with* $f \in W^{1,1}(\mathbb{R}^d)$ *we have that* $J(\Omega)$ *is level set shape differentiable at* Ω *(in the sense of Definition 5.7 with* $\mathcal{X} = W^{2,\infty}(\mathbb{R}^d)$*) with Fréchet derivative* $J'(\Omega)(\eta) = \int_{\partial\Omega} f(\boldsymbol{a})\left(-\eta(\boldsymbol{a})|\nabla\phi(\boldsymbol{a})|^{-1}\right)d\boldsymbol{a}$ *for all* $\eta \in W^{2,\infty}(\mathbb{R}^d)$.

Proof. First note that $\Omega(\phi+\eta) = \Omega_1 = \boldsymbol{\Phi}_1(\Omega_0) \equiv \widetilde{\boldsymbol{\Phi}}(\Omega)$ and $\Omega(\phi) = \Omega_0 \equiv \Omega$. In addition,

$$J'(\Omega(\phi))(\eta) = \int_{\partial\Omega(\phi)} f(\boldsymbol{a})\left(-\frac{\eta(\boldsymbol{a})}{|\nabla\phi(\boldsymbol{a})|}\right)d\boldsymbol{a} = \int_{\partial\Omega} f(\boldsymbol{a})\boldsymbol{V}_\eta(\boldsymbol{a})\cdot\boldsymbol{\nu}\,d\boldsymbol{a} = J'(\Omega)(\boldsymbol{V}_\eta),$$

where $\boldsymbol{V}_\eta$ is given by (5.17). Now, note that

$$\begin{aligned} J(\Omega(\phi+\eta)) &= \int_{\widetilde{\boldsymbol{\Phi}}(\Omega)} f(\boldsymbol{x})d\boldsymbol{x} - \int_{\boldsymbol{\Phi}_\eta(\Omega)} f(\boldsymbol{x})d\boldsymbol{x} + \int_{\boldsymbol{\Phi}_\eta(\Omega)} f(\boldsymbol{x})d\boldsymbol{x} \\ &= \int_{\widetilde{\boldsymbol{\Phi}}(\Omega)} f(\boldsymbol{x})d\boldsymbol{x} - \int_{\boldsymbol{\Phi}_\eta(\Omega)} f(\boldsymbol{x})d\boldsymbol{x} + J(\Omega_{\boldsymbol{V}_\eta}) \\ &= \underbrace{\int_\Omega f(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))\det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))d\boldsymbol{a} - \int_\Omega f(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\det(\nabla_{\boldsymbol{a}}\boldsymbol{\Phi}_\eta(\boldsymbol{a}))d\boldsymbol{a}}_{=T_6} + J(\Omega_{\boldsymbol{V}_\eta}). \end{aligned} \tag{5.31}$$

By the fundamental theorem of calculus, we have

$$f(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a})) - f(\boldsymbol{\Phi}_\eta(\boldsymbol{a})) = \int_0^1 \nabla f\left(s\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}) + (1-s)\boldsymbol{\Phi}_\eta(\boldsymbol{a})\right)\cdot\left(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}) - \boldsymbol{\Phi}_\eta(\boldsymbol{a})\right)ds, \tag{5.32}$$

and so

$$\begin{aligned} |T_6| \le& \int_\Omega \left|f(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a})) - f(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\right|\cdot|\det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))|d\boldsymbol{a} \\ &+ \int_\Omega |f(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))|\cdot\left|\det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a})) - \det(\nabla_{\boldsymbol{a}}\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\right|d\boldsymbol{a} \\ \le& C\|f\|_{W^{1,1}(\mathbb{R}^d)}\|\eta\|^2_{W^{1,\infty}} \\ &+ C\|f\|_{L^1(\mathbb{R}^d)}\left(\|\eta\|^2_{W^{2,\infty}} + \|\phi_k\|_{W^{3,\infty}}\|\eta\|^2_{L^\infty} + \|\phi_k - \phi\|_{W^{2,\infty}}\|\eta\|_{L^\infty}\right), \end{aligned} \tag{5.33}$$

where we used Theorem 5.8 and Corollary 5.9. Therefore,

$$J(\Omega(\phi+\eta)) - J(\Omega(\phi)) - J'(\Omega(\phi))(\eta) = T_6 + J(\Omega_{\boldsymbol{V}_\eta}) - J(\Omega) - J'(\Omega)(\boldsymbol{V}_\eta), \tag{5.34}$$

and since $\|\boldsymbol{V}_\eta\|_{W^{1,\infty}} \leq C_\eta \|\eta\|_{W^{1,\infty}}$, for all $k \geq 1$, we obtain

$$
\begin{aligned}
&\lim_{\|\eta\|_{W^{2,\infty}} \to 0} \frac{|J(\Omega(\phi+\eta)) - J(\Omega(\phi)) - J'(\Omega(\phi))(\eta)|}{\|\eta\|_{W^{2,\infty}}} \\
&\qquad \leq C\|\phi_k - \phi\|_{W^{2,\infty}} + C_\eta \lim_{\|\boldsymbol{V}_\eta\|_{W^{1,\infty}} \to 0} \frac{|J(\Omega_{\boldsymbol{V}_\eta}) - J(\Omega) - J'(\Omega)(\boldsymbol{V}_\eta)|}{\|\boldsymbol{V}_\eta\|_{W^{1,\infty}}} \\
&\qquad \leq C\|\phi_k - \phi\|_{W^{2,\infty}},
\end{aligned}
\tag{5.35}
$$

where we used Theorem 5.5. Taking $k \to \infty$ proves the result. □

5.3. Shape Differentiability on a Cut Subdomain

We now extend the above results to computing shape derivatives when Ω is "cut" by another fixed domain. In other words, consider the shape functional:

$$
J_T(\Omega) = \int_{T\cap\Omega} f(\boldsymbol{x})\, d\boldsymbol{x}, \tag{5.36}
$$

where, again, $f \in W^{1,1}(\mathbb{R}^d)$ and T is a fixed, bounded Lipschitz domain with piecewise smooth boundary. We seek to prove that (5.36) is Fréchet differentiable with respect to Ω keeping T fixed. In Section 5.4, T will correspond to an element in the mesh.

We start by introducing a smooth regularization ρ_ϵ of the characteristic function χ_T with $\epsilon > 0$, that satisfies the following properties:

$$
\rho_\epsilon(\boldsymbol{x}) \to \chi_T(\boldsymbol{x}), \quad \text{for all } \ \boldsymbol{x} \notin \partial T, \quad \|\rho_\epsilon - \chi_T\|_{L^1(\mathbb{R}^d)} \to 0, \quad \text{as } \epsilon \to 0. \tag{5.37}
$$

With this, we define

$$
J_T^\epsilon(\Omega) = \int_\Omega \rho_\epsilon(\boldsymbol{x}) f(\boldsymbol{x})\, d\boldsymbol{x}, \quad \Rightarrow \quad \lim_{\epsilon\to 0} J_T^\epsilon(\Omega) = \int_\Omega \chi_T(\boldsymbol{x}) f(\boldsymbol{x})\, d\boldsymbol{x} = J_T(\Omega). \tag{5.38}
$$

The following assumption is crucial.

Assumption 3. *Assume that $\partial\Omega \cap \partial T$ has vanishing $\mathbb{R}^{d-1}$ Lebesgue measure.*

Under Assumption 3, we have that

$$\chi_{\partial\Omega}(\boldsymbol{x})\rho_\epsilon(\boldsymbol{x}) \to \chi_{\partial\Omega\cap T}(\boldsymbol{x}), \quad \text{for a.e.} \quad \boldsymbol{x} \in \partial\Omega, \quad \text{as } \epsilon \to 0, \tag{5.39}$$

and also

$$\lim_{\epsilon\to 0} \int_{\partial\Omega} \rho_\epsilon(\boldsymbol{x}) g(\boldsymbol{x})\, dS(\boldsymbol{x}) = \int_{\partial\Omega\cap T} g(\boldsymbol{x})\, dS(\boldsymbol{x}), \quad \text{for all} \quad g \in L^1(\partial\Omega). \tag{5.40}$$

5.3.1. Fréchet Differentiability on a Cut Subdomain

Throughout this section, we will assume that Ω is Lipschitz.. We first show the Fréchet differentiability of the shape functional for standard domain perturbations (analogous to Section 5.1). We start with the following lemmas.

Lemma 5.11. *Given $f \in L^1(\mathbb{R}^d)$ and $\boldsymbol{U} \in [W^{1,\infty}(\mathbb{R}^d)]^d$ we have that*

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0} \frac{\int_\Omega \left[f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a}))\chi_T(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})\chi_T(\boldsymbol{a})\right] G(\nabla_{\boldsymbol{a}}\boldsymbol{U}(\boldsymbol{a}))d\boldsymbol{a}}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0, \tag{5.41}$$

where $G : \mathbb{R}^{d\times d} \to \mathbb{R}$ is continuous and $|G(M)| \leq C|M|$ for all $M \in \mathbb{R}^{d\times d}$, for some bounded constant $C > 0$.

Proof. Since $\chi_T \in L^\infty(\mathbb{R}^d)$, then $f \cdot \chi_T \in L^1(\mathbb{R}^d)$. Thus, the result follows from Lemma 5.3. □

Lemma 5.12. *Given $f \in W^{1,1}(\mathbb{R}^d)$ and $\boldsymbol{U} \in [W^{1,\infty}(\mathbb{R}^d)]^d$ we have that*

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0} \lim_{\epsilon\to 0} \frac{\int_\Omega f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})\rho_\epsilon(\boldsymbol{a})d\boldsymbol{a} - \int_\Omega \nabla[f(\boldsymbol{a})\rho_\epsilon(\boldsymbol{a})] \cdot \boldsymbol{U}(\boldsymbol{a})d\boldsymbol{a}}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0, \tag{5.42}$$

provided Assumption 3 holds.

Proof. Let $\epsilon > 0$ be fixed and start by expanding the numerator in (5.42), i.e.

$$\begin{aligned} I_\epsilon(\boldsymbol{U}) &:= \int_\Omega f(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_{\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})\rho_\epsilon(\boldsymbol{a})d\boldsymbol{a} - \int_\Omega \nabla[f(\boldsymbol{a})\rho_\epsilon(\boldsymbol{a})]\cdot \boldsymbol{U}(\boldsymbol{a})d\boldsymbol{a} \\ &= \int_\Omega \int_0^1 \nabla\left[f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\right] ds \cdot \boldsymbol{U}(\boldsymbol{a})d\boldsymbol{a} - \int_\Omega \nabla[f(\boldsymbol{a})\rho_\epsilon(\boldsymbol{a})]\cdot \boldsymbol{U}(\boldsymbol{a})d\boldsymbol{a} \\ &= \int_\Omega \int_0^1 \left[\nabla\left[f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\right] - \nabla[f(\boldsymbol{a})\rho_\epsilon(\boldsymbol{a})]\right]\cdot \boldsymbol{U}(\boldsymbol{a})dsd\boldsymbol{a}, \end{aligned} \tag{5.43}$$

where we used (5.6). Expanding further, we get

$$\begin{aligned} I_\epsilon(\boldsymbol{U}) = &\int_\Omega \int_0^1 \left[\nabla\left[f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\right] - \nabla[f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{a})]\right]\cdot \boldsymbol{U}(\boldsymbol{a})dsd\boldsymbol{a} \\ &+ \int_\Omega \int_0^1 \left[\rho_\epsilon(\boldsymbol{a})\left(\nabla f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f(\boldsymbol{a})\right)\right]\cdot \boldsymbol{U}(\boldsymbol{a})dsd\boldsymbol{a} \\ &+ \int_\Omega \int_0^1 \nabla\cdot\left[\rho_\epsilon(\boldsymbol{a})\left(f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})\right)\boldsymbol{U}(\boldsymbol{a})\right] dsd\boldsymbol{a} \\ &- \int_\Omega \int_0^1 \rho_\epsilon(\boldsymbol{a})\nabla\cdot\left[\left(f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})\right)\boldsymbol{U}(\boldsymbol{a})\right] dsd\boldsymbol{a} \\ =:& A_\epsilon^1 + A_\epsilon^2 + A_\epsilon^3 - A_\epsilon^4. \end{aligned} \tag{5.44}$$

Next, estimate A_ϵ^2. By the Lebesgue dominated convergence theorem and Fubini's Thm. (using Prop. 4.12),

$$\begin{aligned} \lim_{\epsilon\to 0} \frac{|A_\epsilon^2|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} &= \frac{1}{\|\boldsymbol{U}\|_{W^{1,\infty}}} \left| \int_\Omega \chi_T(\boldsymbol{a}) \int_0^1 \left(\nabla f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f(\boldsymbol{a})\right)\cdot \boldsymbol{U}(\boldsymbol{a})dsd\boldsymbol{a} \right| \\ &\leq \frac{1}{\|\boldsymbol{U}\|_{W^{1,\infty}}} \int_0^1 \int_{\Omega\cap T} \left|\nabla f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f(\boldsymbol{a})\right| d\boldsymbol{a}ds \; \|\boldsymbol{U}\|_{L^\infty} \\ &\leq \int_0^1 \int_\Omega \left|\nabla f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \nabla f(\boldsymbol{a})\right| d\boldsymbol{a}ds. \end{aligned} \tag{5.45}$$

We then have

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0} \lim_{\epsilon\to 0} \frac{|A_\epsilon^2|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0, \tag{5.46}$$

by using the same method from (5.8) in the proof of Lemma 5.4. For A_ϵ^3, we apply the divergence theorem:

$$\begin{aligned} \lim_{\epsilon\to 0} A_\epsilon^3 &= \lim_{\epsilon\to 0} \int_0^1 \int_{\partial\Omega} \rho_\epsilon(\boldsymbol{a})\left(f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})\right)\boldsymbol{U}(\boldsymbol{a})\cdot \boldsymbol{\nu}(\boldsymbol{a})dS(\boldsymbol{a})ds \\ &= \int_{\partial\Omega} \chi_T(\boldsymbol{a}) \int_0^1 \left(f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - f(\boldsymbol{a})\right)\boldsymbol{U}(\boldsymbol{a})\cdot \boldsymbol{\nu}(\boldsymbol{a})dsdS(\boldsymbol{a}). \end{aligned} \tag{5.47}$$

Then,

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0}\lim_{\epsilon\to 0}\frac{|A_\epsilon^3|}{\|\boldsymbol{U}\|_{W^{1,\infty}}}\leq \lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0}\int_0^1\int_{\partial\Omega}|f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-f(\boldsymbol{a})|\,dS(\boldsymbol{a})ds=0, \tag{5.48}$$

by a similar argument as for A_ϵ^2 and using a trace theorem. As for A_ϵ^4, we have

$$\lim_{\epsilon\to 0}A_\epsilon^4=\int_\Omega \chi_T(\boldsymbol{a})\int_0^1\nabla\cdot\left[\left(f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-f(\boldsymbol{a})\right)\boldsymbol{U}(\boldsymbol{a})\right]ds d\boldsymbol{a}, \tag{5.49}$$

and so

$$\begin{aligned}
&\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0}\lim_{\epsilon\to 0}\frac{|A_\epsilon^4|}{\|\boldsymbol{U}\|_{W^{1,\infty}}}\\
\leq&\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0}\frac{1}{\|\boldsymbol{U}\|_{W^{1,\infty}}}\int_0^1\int_{\Omega\cap T}\nabla\cdot\left[\left(f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-f(\boldsymbol{a})\right)\boldsymbol{U}(\boldsymbol{a})\right]d\boldsymbol{a}ds\\
\leq&\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0}\int_0^1\int_\Omega\left|\nabla\left(f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-f(\boldsymbol{a})\right)\right|d\boldsymbol{a}ds+\int_0^1\int_\Omega|f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-f(\boldsymbol{a})|\,d\boldsymbol{a}ds\\
\leq&\gamma_1\|f-f_k\|_{W^{1,1}(\mathbb{R}^d)},
\end{aligned} \tag{5.50}$$

for all $k\geq 1$ by using the same method from (5.8) in the proof of Lemma 5.4. Thus,

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0}\lim_{\epsilon\to 0}\frac{|A_\epsilon^4|}{\|\boldsymbol{U}\|_{W^{1,\infty}}}=0.$$

Now, we expand A_ϵ^1:

$$\begin{aligned}
A_\epsilon^1=&\int_0^1\int_\Omega\nabla\cdot\left[f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\left(\rho_\epsilon(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-\rho_\epsilon(\boldsymbol{a})\right)\boldsymbol{U}(\boldsymbol{a})\right]d\boldsymbol{a}ds\\
&-\int_0^1\int_\Omega f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))\left(\rho_\epsilon(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-\rho_\epsilon(\boldsymbol{a})\right)\nabla\cdot\boldsymbol{U}(\boldsymbol{a})d\boldsymbol{a}ds\\
=:&\,B_\epsilon^1-B_\epsilon^2.
\end{aligned} \tag{5.51}$$

By the Lebesgue dominated convergence theorem,

$$\lim_{\epsilon\to 0}\frac{|B_\epsilon^2|}{\|\boldsymbol{U}\|_{W^{1,\infty}}}\leq\int_0^1\int_\Omega|f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))|\,|\chi_T(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-\chi_T(\boldsymbol{a})|\,d\boldsymbol{a}ds. \tag{5.52}$$

For each fixed $\boldsymbol{U}$ and $s\in[0,1]$, let $E_s=\{\boldsymbol{a}\in\mathbb{R}^d:|\chi_T(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-\chi_T(\boldsymbol{a})|=1\}$, and note that $|\chi_T(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))-\chi_T(\boldsymbol{a})|=0$ on $\mathbb{R}^d\setminus E_s$. Also, note that $\chi_T\circ\boldsymbol{\Phi}_{s\boldsymbol{U}}=\chi_{\widetilde{T}}$, i.e. is the characteristic function of $\widetilde{T}=\boldsymbol{\Phi}_{s\boldsymbol{U}}^{-1}(T)$.

A simple argument gives that $E_s \subset \widetilde{E} := (T \setminus \widetilde{T}) \cup (\widetilde{T} \setminus T)$. Set $\delta = s\|\boldsymbol{U}\|_{L^\infty}$. Clearly, $\operatorname{dist}(\boldsymbol{x}, \partial T) \leq \delta$ for all $\boldsymbol{x} \in \widetilde{T} \setminus T$. Moreover, let $\boldsymbol{x} \in T \setminus \widetilde{T}$, so it has a pre-image $\boldsymbol{a} \notin T$ with $\boldsymbol{x} = \boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})$. Since $|\boldsymbol{x} - \boldsymbol{a}| \leq \delta$, and the line segment with endpoints $\boldsymbol{x}$, $\boldsymbol{a}$ intersects ∂T, then $\operatorname{dist}(\boldsymbol{x}, \partial T) \leq \delta$, which holds for all $\boldsymbol{x} \in T \setminus \widetilde{T}$. Therefore, $\operatorname{dist}(\boldsymbol{x}, \partial T) \leq \delta$ for all $\boldsymbol{x} \in \widetilde{E}$.

Let ω_T be the signed distance function to ∂T that is negative inside T. Since ∂T is Lipschitz and piecewise smooth, the level sets $\{\omega_T = c\}$ are Lipschitz and piecewise smooth for all $|c|$ sufficiently small. Clearly,

$$\widetilde{E} \subset \widetilde{S}_\delta := \{\omega_T \geq -\delta\} \cap \{\omega_T \leq \delta\} \equiv \{\omega_T \geq -\delta\} \setminus \{\omega_T > \delta\}.$$

Since the level sets are Lipschitz and piecewise smooth, one can show that $|\widetilde{S}_\delta| \leq \delta C_0$, where C_0 is a bounded constant depending on the perimeter of ∂T. Indeed, by the monotone convergence theorem, $\chi_{\widetilde{S}_\delta} \to \chi_{\partial T}$ as $\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0$.

Returning to (5.52), we find that

$$\begin{aligned} \lim_{\epsilon \to 0} \frac{|B_\epsilon^2|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} &\leq \gamma_2 \|f - f_k\|_{L^1} + \max_{0 \leq s \leq 1} \|f_k \circ \boldsymbol{\Phi}_{s\boldsymbol{U}}\|_{L^\infty} \int_0^1 \int_{E_s} 1 d\boldsymbol{a} ds \\ &\leq \gamma_2 \|f - f_k\|_{L^1} + L_k \int_0^1 \int_{\widetilde{S}_\delta} 1 d\boldsymbol{a} ds \leq \gamma_2 \|f - f_k\|_{L^1} + L_k C_0 \|\boldsymbol{U}\|_{L^\infty}. \end{aligned} \tag{5.53}$$

As before, we get

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0} \lim_{\epsilon \to 0} \frac{|B_\epsilon^2|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0.$$

For B_ϵ^1, we have by the Divergence theorem and the Lebesgue dominated convergence theorem,

$$\lim_{\epsilon \to 0} \frac{|B_\epsilon^1|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} \leq \int_0^1 \int_{\partial \Omega} |f(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a}))| \, |\chi_T(\boldsymbol{\Phi}_{s\boldsymbol{U}}(\boldsymbol{a})) - \chi_T(\boldsymbol{a})| \, dS(\boldsymbol{a}) ds. \tag{5.54}$$

Similar to (5.53), we get

$$\lim_{\epsilon\to 0}\frac{|B_\epsilon^2|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} \le \gamma_3\|f-f_k\|_{W^{1,1}} + \max_{0\le s\le 1}\||\nabla f_k\circ \boldsymbol{\Phi}_{s\boldsymbol{U}}\|_{L^\infty}\int_0^1\int_{E_s\cap\partial\Omega} 1 dS(\boldsymbol{a})ds$$
$$\le \gamma_3\|f-f_k\|_{W^{1,1}} + L_k\int_0^1\int_{\widetilde{S}_\delta\cap\partial\Omega} 1dS(\boldsymbol{a})ds, \tag{5.55}$$

and note that, by the monotone convergence theorem, $\chi_{\widetilde{S}_\delta\cap\partial\Omega}\to\chi_{\partial T\cap\partial\Omega}$ as $\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0$, which yields

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0}\lim_{\epsilon\to 0}\frac{|B_\epsilon^2|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} \le \gamma_3\|f-f_k\|_{W^{1,1}} + L_k|\partial T\cap\partial\Omega|_{d-1}, \tag{5.56}$$

where $|\partial T\cap\partial\Omega|_{d-1}$ is the $\mathbb{R}^{d-1}$ Lebesgue measure of $\partial T\cap\partial\Omega$. Invoking Assumption 3, and taking the limit in k, we obtain

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}}\to 0}\lim_{\epsilon\to 0}\frac{|B_\epsilon^2|}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0.$$

The proof of (5.42) is complete. □

Theorem 5.13. *Given the shape functional $J_T(\Omega) := \int_{\Omega\cap T} f(\boldsymbol{x})d\boldsymbol{x}$ with $f\in W^{1,1}(\mathbb{R}^d)$ we have that $J_T(\Omega)$ is shape differentiable at Ω (in the sense of Definition 5.1) with Fréchet derivative $J_T'(\Omega)(\boldsymbol{U}) = \int_{\partial\Omega\cap T} f(\boldsymbol{a})\boldsymbol{U}(\boldsymbol{a})\cdot\boldsymbol{\nu}(\boldsymbol{a})dS(\boldsymbol{a})$ for all $\boldsymbol{U}\in[W^{1,\infty}(\mathbb{R}^d)]^d$, provided Assumption 3 holds.*

Proof. Set $A_T(\boldsymbol{U}) := J_T'(\Omega)(\boldsymbol{U})$, let $\epsilon > 0$ be fixed, and define

$$A_T^\epsilon(\boldsymbol{U}) := \int_{\partial\Omega}\rho_\epsilon(\boldsymbol{a})f(\boldsymbol{a})\boldsymbol{U}(\boldsymbol{a})\cdot\boldsymbol{\nu}(\boldsymbol{a})dS(\boldsymbol{a}),$$

where $A_T^\epsilon(\boldsymbol{U}) \to A_T(\boldsymbol{U})$ by (5.40). Using (5.3), we have

$$\begin{aligned}
J_T^\epsilon(\Omega_{\boldsymbol{U}}) - J_T^\epsilon(\Omega) &= \int_{\Omega_{\boldsymbol{U}}} \rho_\epsilon(\boldsymbol{x}) f(\boldsymbol{x}) d\boldsymbol{x} - \int_\Omega \rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a}) d\boldsymbol{a} \\
&= \int_\Omega \rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) \det(I + \nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})) d\boldsymbol{a} - \int_\Omega \rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a}) d\boldsymbol{a} \\
&= \int_\Omega \rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) - \rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a}) d\boldsymbol{a} \\
&\quad + \int_\Omega \rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) \mathrm{tr}(\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})) d\boldsymbol{a} \\
&\quad + \int_\Omega \rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) O(|\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})|^2) d\boldsymbol{a}.
\end{aligned} \tag{5.57}$$

Continuing, we get

$$\begin{aligned}
J_T^\epsilon(\Omega_{\boldsymbol{U}}) - J_T^\epsilon(\Omega) &= \int_\Omega \rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) - \rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a}) d\boldsymbol{a} \\
&\quad - \int_\Omega \nabla_{\boldsymbol{a}} \left(\rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a})\right) \cdot \boldsymbol{U}(\boldsymbol{a}) d\boldsymbol{a} \\
&\quad + \int_\Omega \left[\rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) - \rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a})\right] \nabla_{\boldsymbol{a}} \cdot \boldsymbol{U}(\boldsymbol{a}) d\boldsymbol{a} \\
&\quad + \int_\Omega \left[\rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a}) \nabla_{\boldsymbol{a}} \cdot \boldsymbol{U}(\boldsymbol{a}) + \nabla_{\boldsymbol{a}} \left(\rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a})\right) \cdot \boldsymbol{U}(\boldsymbol{a})\right] d\boldsymbol{a} \\
&\quad + \int_\Omega \rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) O(|\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})|^2) d\boldsymbol{a}.
\end{aligned} \tag{5.58}$$

By Gauss' divergence theorem, we arrive at

$$\begin{aligned}
J_T^\epsilon(\Omega_{\boldsymbol{U}}) - J_T^\epsilon(\Omega) - A_T^\epsilon(\boldsymbol{U}) &= \int_\Omega \rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) - \rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a}) d\boldsymbol{a} \\
&\quad - \int_\Omega \nabla_{\boldsymbol{a}} \left(\rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a})\right) \cdot \boldsymbol{U}(\boldsymbol{a}) d\boldsymbol{a} \\
&\quad + \int_\Omega \left[\rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) - \rho_\epsilon(\boldsymbol{a}) f(\boldsymbol{a})\right] \nabla_{\boldsymbol{a}} \cdot \boldsymbol{U}(\boldsymbol{a}) d\boldsymbol{a} \\
&\quad + \int_\Omega \rho_\epsilon(\boldsymbol{\Phi_U}(\boldsymbol{a})) f(\boldsymbol{\Phi_U}(\boldsymbol{a})) O(|\nabla_{\boldsymbol{a}} \boldsymbol{U}(\boldsymbol{a})|^2) d\boldsymbol{a}.
\end{aligned} \tag{5.59}$$

Then, by Lemmas 5.11, 5.12, we find that

$$\lim_{\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0} \frac{J_T(\Omega_{\boldsymbol{U}}) - J_T(\Omega) - J_T'(\Omega)(\boldsymbol{U})}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = \lim_{\|\boldsymbol{U}\|_{W^{1,\infty}} \to 0} \lim_{\epsilon \to 0} \frac{J_T^\epsilon(\Omega_{\boldsymbol{U}}) - J_T^\epsilon(\Omega) - A_T^\epsilon(\boldsymbol{U})}{\|\boldsymbol{U}\|_{W^{1,\infty}}} = 0, \tag{5.60}$$

which proves the assertion. □

5.3.2. Level Set Fréchet Differentiability on a Cut Subdomain

In this section, we will assume that the level set function ϕ for Ω is in $W^{2,\infty}(\mathbb{R}^d)$, hence Ω is better than Lipschitz and is in fact $C^{1,1}$. We now prove the cut version of Theorem 5.10.

Theorem 5.14. *Adopt the hypothesis of Theorem 5.13. Assume $\phi \in W^{2,\infty}(\mathbb{R}^d)$ and that it satisfies Definition 5.6 for some positive constants c_0, δ_0. Let $\Omega(\phi+\eta)$ be the sub-zero level set of $\phi+\eta$. Then, $J_T(\Omega)$ is level set shape differentiable at Ω (in the sense of Definition 5.7) with Fréchet derivative $J'_T(\Omega)(\eta) = \int_{\partial\Omega\cap T} f(\boldsymbol{a})\,(-\eta(\boldsymbol{a})|\nabla\phi(\boldsymbol{a})|^{-1})\,d\boldsymbol{a}$ for all $\eta \in [W^{2,\infty}(\mathbb{R}^d)]^d$.*

Proof. Recall that $\boldsymbol{\Phi}_t$ in (5.10) is different from $\boldsymbol{\Phi}_\eta$ in (5.17). We first note that $\Omega(\phi+\eta) = \Omega_1 = \boldsymbol{\Phi}_1(\Omega_0) \equiv \widetilde{\boldsymbol{\Phi}}(\Omega)$ and $\Omega(\phi) = \Omega_0 \equiv \Omega$. In addition,

$$J'_T(\Omega(\phi))(\eta) = \int_{\partial\Omega(\phi)\cap T} f(\boldsymbol{a}) \left(-\frac{\eta(\boldsymbol{a})}{|\nabla\phi(\boldsymbol{a})|} \right) d\boldsymbol{a} = \int_{\partial\Omega\cap T} f(\boldsymbol{a}) \boldsymbol{V}_\eta(\boldsymbol{a}) \cdot \boldsymbol{\nu}\, d\boldsymbol{a} = J'_T(\Omega)(\boldsymbol{V}_\eta),$$

where $\boldsymbol{V}_\eta$ is given by (5.17). Now, note that

$$\begin{aligned}
&J_T(\Omega(\phi+\eta)) \\
&\quad = \int_{\widetilde{\boldsymbol{\Phi}}(\Omega)\cap T} f(\boldsymbol{x})d\boldsymbol{x} - \int_{\boldsymbol{\Phi}_\eta(\Omega)\cap T} f(\boldsymbol{x})d\boldsymbol{x} + \int_{\boldsymbol{\Phi}_\eta(\Omega)\cap T} f(\boldsymbol{x})d\boldsymbol{x} \\
&\quad = \lim_{\epsilon\to 0} \int_{\widetilde{\boldsymbol{\Phi}}(\Omega)} f(\boldsymbol{x})\rho_\epsilon(\boldsymbol{x})d\boldsymbol{x} - \int_{\boldsymbol{\Phi}_\eta(\Omega)} f(\boldsymbol{x})\rho_\epsilon(\boldsymbol{x})d\boldsymbol{x} + J_T(\Omega_{\boldsymbol{V}_\eta}) \\
&\quad = \lim_{\epsilon\to 0} \underbrace{\int_\Omega f(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))\rho_\epsilon(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))\det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))d\boldsymbol{a} - \int_\Omega f(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\det(\nabla_{\boldsymbol{a}}\boldsymbol{\Phi}_\eta(\boldsymbol{a}))d\boldsymbol{a}}_{=Z_\epsilon} \\
&\qquad\quad + J(\Omega_{\boldsymbol{V}_\eta}).
\end{aligned}$$

Next, we split the Z_ϵ term:

$$
\begin{aligned}
Z_\epsilon &= Q_\epsilon^1 + Q_\epsilon^2, \\
Q_\epsilon^1 &= \int_\Omega f(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_\eta(\boldsymbol{a})) \left(\det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a})) - \det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))\right) d\boldsymbol{a} \\
Q_\epsilon^2 &= \int_\Omega \left(f(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))\rho_\epsilon(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a})) - f(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\right) \det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))d\boldsymbol{a}.
\end{aligned}
\tag{5.61}
$$

Estimating Q_ϵ^1 is similar to (5.33), i.e. we have

$$
\lim_{\epsilon\to 0}|Q_\epsilon^1| \le C\|f\|_{L^1(\mathbb{R}^d)} \left(\|\eta\|_{W^{2,\infty}}^2 + \|\phi_k\|_{W^{3,\infty}}\|\eta\|_{L^\infty}^2 + \|\phi_k - \phi\|_{W^{2,\infty}}\|\eta\|_{L^\infty}\right). \tag{5.62}
$$

As for Q_ϵ^2, we have the following:

$$
\begin{aligned}
Q_\epsilon^2 &= \int_\Omega \left(f(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))\rho_\epsilon(\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a})) - f(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\rho_\epsilon(\boldsymbol{\Phi}_\eta(\boldsymbol{a}))\right) \det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))d\boldsymbol{a} \\
&= \int_\Omega\int_0^1 \nabla(f\rho_\epsilon)\circ(t\widetilde{\boldsymbol{\Phi}} + (1-t)\boldsymbol{\Phi}_\eta)\cdot(\widetilde{\boldsymbol{\Phi}} - \boldsymbol{\Phi}_\eta)\det(\nabla_{\boldsymbol{a}}\widetilde{\boldsymbol{\Phi}}(\boldsymbol{a}))dtd\boldsymbol{a} \\
|Q_\epsilon^2| &\lesssim \int_\Omega\int_0^1 \left|\nabla(f\rho_\epsilon)\circ(t\widetilde{\boldsymbol{\Phi}} + (1-t)\boldsymbol{\Phi}_\eta)\cdot(\widetilde{\boldsymbol{\Phi}} - \boldsymbol{\Phi}_\eta)\right| dtd\boldsymbol{a} \\
&\le \int_0^1\int_\Omega \left|\nabla\cdot\left[(f\rho_\epsilon)\circ(t\widetilde{\boldsymbol{\Phi}} + (1-t)\boldsymbol{\Phi}_\eta)(\widetilde{\boldsymbol{\Phi}} - \boldsymbol{\Phi}_\eta)\right]\right| dtd\boldsymbol{a} \\
&\quad + \int_0^1\int_\Omega \left|(f\rho_\epsilon)\circ(t\widetilde{\boldsymbol{\Phi}} + (1-t)\boldsymbol{\Phi}_\eta)\right| \left|\nabla\cdot(\widetilde{\boldsymbol{\Phi}} - \boldsymbol{\Phi}_\eta)\right| dtd\boldsymbol{a},
\end{aligned}
\tag{5.63}
$$

where we have used the fundamental theorem for line integrals. Note that we have the following estimate as a consequence of Theorem 5.8

$$
\begin{aligned}
&\lim_{\epsilon\to 0}\int_0^1\int_\Omega \left|(f\rho_\epsilon)\circ(t\widetilde{\boldsymbol{\Phi}} + (1-t)\boldsymbol{\Phi}_\eta)\right| \left|\nabla\cdot(\widetilde{\boldsymbol{\Phi}} - \boldsymbol{\Phi}_\eta)\right| dtd\boldsymbol{a} \\
&\qquad \lesssim \|f\|_{L^1(\mathbb{R}^d)} \left(\|\eta\|_{W^{2,\infty}}^2 + \|\phi_k\|_{W^{3,\infty}}\|\eta\|_{L^\infty}^2 + \|\phi_k - \phi\|_{W^{2,\infty}}\|\eta\|_{L^\infty}\right).
\end{aligned}
\tag{5.64}
$$

Now we use the divergence theorem and Theorem 5.8 on the remaining term to get the following estimate.

$$
\begin{aligned}
&\lim_{\epsilon\to 0}\int_0^1\int_\Omega \left|\nabla\cdot\left[(f\rho_\epsilon)\circ(t\widetilde{\boldsymbol{\Phi}} + (1-t)\boldsymbol{\Phi}_\eta)(\widetilde{\boldsymbol{\Phi}} - \boldsymbol{\Phi}_\eta)\right]\right| dtd\boldsymbol{a} \\
\lesssim &\lim_{\epsilon\to 0}\int_0^1\int_{\partial\Omega} \left|(f\rho_\epsilon)\circ(t\widetilde{\boldsymbol{\Phi}} + (1-t)\boldsymbol{\Phi}_\eta)(\widetilde{\boldsymbol{\Phi}} - \boldsymbol{\Phi}_\eta)\right| dtd\boldsymbol{a} \\
\lesssim &\|f\|_{W^{1,1}(\mathbb{R}^d)}\|\eta\|_{W^{2,\infty}}^2.
\end{aligned}
\tag{5.65}
$$

Hence,

$$\lim_{\epsilon\to 0}|Z_\epsilon| \lesssim \|f\|_{W^{1,1}(\mathbb{R}^d)}\left(\|\eta\|^2_{W^{2,\infty}} + \|\phi_k\|_{W^{3,\infty}}\|\eta\|^2_{L^\infty} + \|\phi_k-\phi\|_{W^{2,\infty}}\|\eta\|_{L^\infty}\right). \tag{5.66}$$

Therefore,

$$J_T(\Omega(\phi+\eta)) - J_T(\Omega(\phi)) - J_T'(\Omega(\phi))(\eta) = \lim_{\epsilon\to 0} Z_\epsilon + J_T(\Omega_{\boldsymbol{V}_\eta}) - J_T(\Omega) - J_T'(\Omega)(\boldsymbol{V}_\eta), \tag{5.67}$$

and since $\|\boldsymbol{V}_\eta\|_{W^{1,\infty}} \leq C_\eta\|\eta\|_{W^{1,\infty}}$, for all $k \geq 1$, we obtain

$$\begin{aligned}
&\lim_{\|\eta\|_{W^{2,\infty}}\to 0} \frac{|J_T(\Omega(\phi+\eta)) - J_T(\Omega(\phi)) - J_T'(\Omega(\phi))(\eta)|}{\|\eta\|_{W^{2,\infty}}} \\
&\qquad \leq C\|\phi_k-\phi\|_{W^{2,\infty}} + C_\eta \lim_{\|\boldsymbol{V}_\eta\|_{W^{1,\infty}}\to 0} \frac{|J_T(\Omega_{\boldsymbol{V}_\eta}) - J_T(\Omega) - J_T'(\Omega)(\boldsymbol{V}_\eta)|}{\|\boldsymbol{V}_\eta\|_{W^{1,\infty}}} \\
&\qquad \leq C\|\phi_k-\phi\|_{W^{2,\infty}},
\end{aligned} \tag{5.68}$$

where we used Theorem 5.13. Taking $k\to\infty$ proves the result. □

5.4. Shape Fréchet Differentiability over a Mesh

We now consider piecewise defined functions over the mesh $\widehat{\mathcal{T}}_h$. In particular, on $\widehat{\mathcal{T}}_h$, define:

$$\mathcal{W}_h = \{w_h \in L^1(\widehat{\mathfrak{D}}) : w_h|_T \in W^{1,1}(T),\ \forall T \in \widehat{\mathcal{T}}_h\}, \tag{5.69}$$

with norm given by

$$\|w_h\|_{\mathcal{W}_h} := \|w_h\|_{L^1(\widehat{\mathfrak{D}})} + \sum_{T\in\widehat{\mathcal{T}}_h} \|\nabla w_h\|_{L^1(T)} + \sum_{F\in\widehat{\mathcal{F}}_h^0} \|\,[\![w_h]\!]\,\|_{L^1(F)}. \tag{5.70}$$

By using the previous results, we can generalize Theorem 5.5 to allow for functions in $\mathcal{W}_h$. To this end, we need a global mesh version of Assumption 3.

Assumption 4. *Assume that $\partial\Omega\cap\partial T$ has vanishing $\mathbb{R}^{d-1}$ Lebesgue measure for all $T \in \widehat{\mathcal{T}}_h$.*

Theorem 5.15. *For the shape functional $J(\Omega) := \int_\Omega f_h(\boldsymbol{x})d\boldsymbol{x}$ with $f_h \in \mathcal{W}_h$ we have that $J(\Omega)$ is shape differentiable at Ω (in the sense of Definition 5.1) with Fréchet derivative $J'(\Omega)(\boldsymbol{U}) = \int_{\partial\Omega} f_h(\boldsymbol{a})\boldsymbol{U}(\boldsymbol{a}) \cdot \boldsymbol{\nu}(\boldsymbol{a})d\boldsymbol{a}$ for all $\boldsymbol{U} \in [W^{1,\infty}(\mathbb{R}^d)]^d$, provided Assumption 4 holds.*

Proof. First, note that $f_h|_T \in W^{1,1}(T)$ for all $T \in \widehat{\mathcal{T}}_h$. Let $f_T : \mathbb{R}^d \to \mathbb{R}$ be a bounded extension of $f_h|_T$ to $W^{1,1}(\mathbb{R}^d)$, for all $T \in \widehat{\mathcal{T}}_h$. Then,

$$J(\Omega_{\boldsymbol{U}}) - J(\Omega) - J'(\Omega)(\boldsymbol{U}) = \sum_{T\in\widehat{\mathcal{T}}_h} J_T(\Omega_{\boldsymbol{U}}) - J_T(\Omega) - J'_T(\Omega)(\boldsymbol{U}),$$

where

$$J_T(\Omega) = \int_{\Omega\cap T} f_T(\boldsymbol{a})d\boldsymbol{a}, \quad J'_T(\Omega)(\boldsymbol{U}) = \int_{\partial\Omega\cap T} f_T(\boldsymbol{a})\boldsymbol{U}(\boldsymbol{a}) \cdot \boldsymbol{\nu}(\boldsymbol{a})d\boldsymbol{a}. \tag{5.71}$$

For each term in the sum, one can apply Theorem 5.13. Since the sum is finite, we easily obtain the Fréchet shape differentiability of $J(\Omega)$. □

Next, we consider domains defined using the space $\mathcal{B}_h$ given in Section 3.1. Thus, let $\Omega(\phi_h)$ be the sub-zero level set of ϕ_h, where $\phi_h \in \mathcal{B}_h$ and satisfies Definition 5.6 for some positive constants c_0, δ_0. We will show that $J(\Omega(\phi_h))$ is level set shape Fréchet differentiable in the sense of Definition 5.7 with $\mathcal{X} = \mathcal{B}_h$.

Theorem 5.16. *Assume $\phi_h \in \mathcal{B}_h$ satisfies Definition 5.6 for some positive constants c_0, δ_0. For the shape functional $J(\Omega(\phi_h)) := \int_{\Omega(\phi_h)} f_h(\boldsymbol{x})d\boldsymbol{x}$ with $f_h \in \mathcal{W}_h$, we have that $J(\Omega(\phi_h))$ is level set shape differentiable at $\Omega(\phi_h)$ (in the sense of Definition 5.7 with $\mathcal{X} = \mathcal{B}_h$) with Fréchet derivative $J'(\Omega(\phi_h))(\eta_h) = \int_{\partial\Omega(\phi_h)} f_h(\boldsymbol{a}) \left(-\eta_h(\boldsymbol{a})|\nabla\phi_h(\boldsymbol{a})|^{-1}\right) d\boldsymbol{a}$ for all $\eta_h \in \mathcal{B}_h$, provided Assumption 4 holds.*

Proof. We proceed similarly to the proof of Theorem 5.15. Let $f_T : \mathbb{R}^d \to \mathbb{R}$ be a bounded extension of $f_h|_T$ to $W^{1,1}(\mathbb{R}^d)$, for all $T \in \widehat{\mathcal{T}}_h$. Moreover, let $\phi_T : \mathbb{R}^d \to \mathbb{R}$ be a bounded extension of $\phi_h|_T$ to $W^{2,\infty}(\mathbb{R}^d)$, for all $T \in \widehat{\mathcal{T}}_h$; similarly, do a piecewise extension for η_h to $\{\eta_T\} \subset W^{2,\infty}(\mathbb{R}^d)$. See [71, Sec. VI.3.1] for details of the extension. Then,

$$\begin{aligned} &J(\Omega(\phi_h + \eta_h)) - J(\Omega(\phi_h)) - J'(\Omega(\phi_h))(\eta_h) \\ &\qquad = \sum_{T \in \widehat{\mathcal{T}}_h} J_T(\Omega(\phi_T + \eta_T)) - J_T(\Omega(\phi_T)) - J'_T(\Omega(\phi_T))(\eta_T), \end{aligned}$$

where

$$J_T(\Omega(\phi_T)) = \int_{\Omega(\phi_T)\cap T} f_T(\boldsymbol{a}) d\boldsymbol{a}, \quad J'_T(\Omega(\phi_T))(\eta_T) = \int_{\partial\Omega(\phi_T)\cap T} f_T(\boldsymbol{a}) \left(-\frac{\eta_T}{|\nabla \phi_T(\boldsymbol{a})|} \right) d\boldsymbol{a}. \tag{5.72}$$

For each term in the sum, one can apply Theorem 5.14. Since the sum is finite, we easily obtain the Fréchet shape differentiability of $J(\Omega(\phi_h))$. □

5.5. When the Boundary Intersects a Facet

We now consider the case where Assumption 4 is violated. Suppose the violation happens on a single facet $F = \overline{T_+} \cap \overline{T_-}$ where $E := \partial\Omega \cap \partial T \subset F$ with $|E|_{d-1} > 0$. On E, $|\boldsymbol{\nu} \cdot \boldsymbol{n}| = 1$ where $\boldsymbol{n}$ is the outer normal of ∂T_+. Then, one can obtain the following modification of Theorem 5.15:

$$\begin{aligned} J'(\Omega)(\boldsymbol{U}) = &\int_{\partial\Omega\setminus E} f_h \boldsymbol{U} \cdot \boldsymbol{\nu} dS + \int_E f_{h,+} \left(\frac{1 - \operatorname{sgn}(\boldsymbol{U} \cdot \boldsymbol{n})}{2} \right) \boldsymbol{U} \cdot \boldsymbol{n} \, dS \\ &+ \int_E f_{h,-} \left(\frac{1 + \operatorname{sgn}(\boldsymbol{U} \cdot \boldsymbol{n})}{2} \right) \boldsymbol{U} \cdot \boldsymbol{n} \, dS, \end{aligned} \tag{5.73}$$

where $f_{h,\pm}$ is the restriction of f_h from $T_\pm$. Note that (5.73) is not a Fréchet derivative, or even a Gâteaux derivative, because (5.73) is not linear in $\boldsymbol{U}$; hence, we refer to (5.73) as the first variation of $J(\Omega)$. If f_h is continuous across the mesh, then (5.73) reduces the Fréchet derivative in Thm. 5.15.

The corresponding modification of Theorem 5.16 is given by

$$\begin{aligned} J'(\Omega)(\boldsymbol{U}) = -\int_{\partial\Omega\setminus E} f_h \frac{\eta_h}{|\nabla\phi_h|} dS + \int_E \frac{f_{h,+}}{|\nabla\phi_{h,+}|}\left(\frac{1+\operatorname{sgn}(\eta_h(\nabla\phi_h\cdot\boldsymbol{n}))}{2}\right)\eta_h\, dS \\ + \int_E \frac{f_{h,-}}{|\nabla\phi_{h,-}|}\left(\frac{1-\operatorname{sgn}(\eta_h(\nabla\phi_h\cdot\boldsymbol{n}))}{2}\right)\eta_h\, dS, \end{aligned} \tag{5.74}$$

where we have assumed that $\operatorname{sgn}(\nabla\phi_{h,+}\cdot\boldsymbol{n}) = \operatorname{sgn}(\nabla\phi_{h,-}\cdot\boldsymbol{n})$ on E with $\phi_{h,\pm}$ denoting the restriction of ϕ_h from $T_\pm$. If f_h *and* $\nabla\phi_h$ are continuous across the mesh, then (5.74) reduces the Fréchet derivative in Thm. 5.16.

In Section 7.3, we illustrate the effect of the discontinuous derivative at facets with a numerical example.

Chapter 6. Unfitted Shape Optimization

We consider a discrete form of the optimization problem discussed in Section 2.1 using the unfitted formulation in (3.21). Furthermore, we develop a gradient descent optimization method to find discrete minimizers using the level set shape derivative formulas derived earlier.

6.1. Admissible Set

The domain Ω_h is parameterized by a level set function $\phi_h \in B_h$. Thus, in principle, we seek to minimize a shape functional $J(\Omega_h)$ over the set of admissible shapes

$$\widetilde{\mathcal{A}}_h = \{\varphi_h \in B_h : c^{-1} \geq |\nabla \varphi_h| \geq c\}, \tag{6.1}$$

for some suitable constant $c > 0$, where the inequality constraints are needed to ensure the domain does not degenerate. Unfortunately, $\widetilde{\mathcal{A}}_h$ is not a convex set.

Therefore, we define a localized admissible set, that is convex, in order to pose a well-defined minimization problem. Suppose we have a given domain Ω_h that is represented through the level set function $\phi_h \in \widetilde{\mathcal{A}}_h$. Next, define:

$$\mathcal{C}(\Sigma) = \{\varphi_h \in B_h : |\nabla \varphi_h| \leq c/2,\, \varphi_h|_\Sigma = 0\}, \tag{6.2}$$

where $\Sigma \subset \partial\widehat{\mathfrak{D}}$, which may be empty, is used to impose additional design constraints in

Figure 6.1. Example of the level set constraint set $\Sigma \subset \partial\widehat{\mathfrak{D}}$ that is denoted by the solid lines.

our optimization (see Figure 6.1). We now verify that $\mathcal{C}$ is a convex set. Let $\varphi_h, \psi_h \in \mathcal{C}$ and $\lambda \in [0,1]$. Then,

$$
\begin{aligned}
|\nabla [\lambda\varphi_h + (1-\lambda)\psi_h]| &= |\lambda\nabla\varphi_h + (1-\lambda)\nabla\psi_h| \\
&\leq \lambda|\nabla\varphi_h| + (1-\lambda)|\nabla\psi_h| \\
&\leq \lambda c/2 + (1-\lambda)c/2 = c/2,
\end{aligned}
$$

i.e. $\lambda\varphi_h+(1-\lambda)\psi_h \in \mathcal{C}$ for all $\varphi_h, \psi_h \in \mathcal{C}$ and all $\lambda \in [0,1]$. Now, define the local admissible set $\mathcal{A}_h(\phi_h, \Sigma) = \{\phi_h\} + \mathcal{C}(\Sigma)$, where ϕ_h is a given *reference* level set function, and note that any $\psi_h \in \mathcal{A}_h(\phi_h, \Sigma)$ satisfies $\psi_h = \phi_h + \varphi_h$, for some $\varphi_h \in \mathcal{C}(\Sigma)$ and

$$
\begin{aligned}
|\nabla\phi_h + \nabla\varphi_h| \geq ||\nabla\phi_h| - |\nabla\varphi_h|| &= |\nabla\phi_h| - |\nabla\varphi_h| \\
&\geq c - c/2 > c/2 > 0.
\end{aligned}
$$

Ergo, any $\psi_h \in \mathcal{A}_h(\phi_h, \Sigma)$ parameterizes a well-defined domain as its sub-zero level set. In our computations, we iteratively update the convex set $\mathcal{A}_h(\cdot, \Sigma)$ in our gradient descent procedure (see Section 6.4).

In practice, we do not allow $|\nabla\phi_h|$ to become close to 0 during the optimization. In fact, we strive to maintain $|\nabla\phi_h| \approx 1$ or at least $|\nabla\phi_h| \geq \frac{1}{2}$. Then, the constraint in (6.2) corresponds to $|\nabla\varphi_h| \leq 1/4$. During the optimization, we periodically reinitialize ϕ_h so that it is close to a signed distance function having the same zero level set as before (see Section 6.4).

6.2. Discrete Optimization Problem

For any $\boldsymbol{v}_h \in V_h(\Omega_h(\phi_h))$, let $J(\phi_h; \boldsymbol{v}_h) \equiv J(\Omega_h(\phi_h); \boldsymbol{v}_h)$ be the shape (cost) functional in (2.12). For a given reference domain $\Omega_h(\widehat{\phi}_h)$, with reference level set function $\widehat{\phi}_h$, consider the following minimization problem

$$J\left(\phi_{h,\min};\boldsymbol{u}_h(\phi_{h,\min})\right) = \min_{\phi_h\in\mathcal{A}_h(\widehat{\phi}_h,\Sigma)} \min_{\boldsymbol{u}_h\in V_h(\Omega_h(\phi_h))} J\left(\phi_h;\boldsymbol{u}_h\right), \tag{6.3}$$
$$\text{subject to } \boldsymbol{u}_h \text{ solving (3.21) on } \Omega_h(\phi_h),$$

where $\boldsymbol{u}_h(\phi_h) \equiv \boldsymbol{u}_h(\Omega_h(\phi_h))$. Since B_h is finite dimensional, $\mathcal{A}_h(\widehat{\phi}_h,\Sigma)$ effectively enforces a bounded Lipschitz constant on the domains it contains; thus, $\mathcal{A}_h(\widehat{\phi}_h,\Sigma)$ has enough compactness to ensure existence of a minimizer (see [1]).

We rewrite the minimization problem using a Lagrangian to free the PDE-constraint, i.e. for any $\phi_h \in \mathcal{A}_h(\widehat{\phi}_h,\Sigma)$, define

$$L\left(\phi_h;\boldsymbol{v}_h,\boldsymbol{q}_h\right) := J\left(\phi_h;\boldsymbol{v}_h\right) - A_h\left(\Omega_h(\phi_h);\boldsymbol{v}_h,\boldsymbol{q}_h\right) + \chi_h\left(\Omega_h(\phi_h);\boldsymbol{q}_h\right), \quad \forall\,\boldsymbol{v}_h,\boldsymbol{q}_h \in B_h, \tag{6.4}$$

and note that by (3.21) the following property holds

$$J\left(\phi_h;\boldsymbol{u}_h(\phi_h)\right) = L\left(\phi_h;\boldsymbol{u}_h(\phi_h),\boldsymbol{q}_h\right),\ \forall \boldsymbol{q}_h \in V_h(\Omega_h(\phi_h)), \tag{6.5}$$

for any $\phi_h \in \widetilde{\mathcal{A}}_h$. The Lagrangian framework allows us to characterize the minimizer in (6.3) as a saddle-point, i.e.

$$L\left(\bar{\phi}_h;\bar{\boldsymbol{u}}_h,\bar{\boldsymbol{p}}_h\right) = \min_{\phi_h\in\mathcal{A}_h(\widehat{\phi}_h,\Sigma)} \min_{\boldsymbol{u}_h\in V_h(\Omega_h(\phi_h))} \max_{\boldsymbol{q}_h\in V_h(\Omega_h(\phi_h))} L\left(\phi_h;\boldsymbol{u}_h,\boldsymbol{q}_h\right), \tag{6.6}$$

for some $\bar{\phi}_h = \widehat{\phi}_h + \bar{q}_h$ with $\bar{q}_h \in \mathcal{C}(\Sigma)$, $\bar{\boldsymbol{u}}_h \in V_h(\bar{\Omega}_h)$, and $\bar{\boldsymbol{p}}_h \in V_h(\bar{\Omega}_h)$, where $\bar{\Omega}_h \equiv \bar{\Omega}_h(\bar{\phi}_h)$. Since L is Fréchet differentiable, with $\delta_a L\left(\Omega;\boldsymbol{v},\boldsymbol{q}\right)(\cdot)$ denoting the Fréchet derivative with respect to the argument a, the following first order conditions must hold for $\bar{\boldsymbol{u}}_h$ and $\bar{\boldsymbol{p}}_h$:

$$\begin{aligned} \delta_{\boldsymbol{q}_h} L\left(\bar{\phi}_h;\bar{\boldsymbol{u}}_h,\bar{\boldsymbol{p}}_h\right)(\boldsymbol{z}_h) = 0,\ \forall \boldsymbol{z}_h \in V_h(\bar{\Omega}_h), \\ \delta_{\boldsymbol{v}_h} L\left(\bar{\phi}_h;\bar{\boldsymbol{u}}_h,\bar{\boldsymbol{p}}_h\right)(\boldsymbol{w}_h) = 0,\ \forall \boldsymbol{w}_h \in V_h(\bar{\Omega}_h), \end{aligned} \tag{6.7}$$

which implies that $\bar{\boldsymbol{u}}_h$ and $\bar{\boldsymbol{p}}_h$ solve the following variational problems

$$\begin{aligned} A_h\left(\bar{\Omega}_h(\bar{\phi}_h); \bar{\boldsymbol{u}}_h, \boldsymbol{v}_h\right) &= \chi_h\left(\bar{\Omega}_h(\bar{\phi}_h); \boldsymbol{v}_h\right), \ \forall \boldsymbol{v}_h \in V_h(\bar{\Omega}_h), \\ A_h\left(\bar{\Omega}_h(\bar{\phi}_h); \boldsymbol{w}_h, \bar{\boldsymbol{p}}_h\right) &= \delta_{\boldsymbol{v}_h} J\left(\bar{\phi}_h; \bar{\boldsymbol{u}}_h\right)(\boldsymbol{w}_h), \ \forall \boldsymbol{w}_h \in V_h(\bar{\Omega}_h). \end{aligned} \tag{6.8}$$

Thus, $\bar{\phi}_h = \phi_{h,\min}$, $\bar{\Omega}_h = \Omega_{h,\min}$, $\bar{\boldsymbol{u}}_h = \boldsymbol{u}_h(\phi_{h,\min})$ solves (3.21) on $\Omega_{h,\min}$, and $\bar{\boldsymbol{p}}_h = \boldsymbol{p}_h(\phi_{h,\min})$ solves an adjoint problem. In addition, we have the following first order condition for $\bar{\phi}_h$:

$$L'\left(\bar{\phi}_h; \bar{\boldsymbol{u}}_h, \bar{\boldsymbol{p}}_h\right)(r_h - \bar{q}_h) \geq 0, \quad \forall\, r_h \in \mathcal{C}(\Sigma). \tag{6.9}$$

6.3. Reduced Gradient

Note that, ultimately, we are after the derivative of the *reduced functional* $\mathcal{J}(\phi_h) := J(\phi_h; \boldsymbol{u}_h(\phi_h))$ in (6.5), i.e. we seek to compute the level set shape derivative $\mathcal{J}'(\phi_h)(\eta_h) \equiv J'(\phi_h; \boldsymbol{u}(\phi_h))(\eta_h)$, so that we can perform gradient based optimization. This is given by the Correa-Seeger theorem [22, pg. 427]:

$$\mathcal{J}'(\phi_h)(\eta_h) = L'(\phi_h; \bar{\boldsymbol{u}}_h(\phi_h), \bar{\boldsymbol{p}}_h(\phi_h))(\eta_h), \quad \forall\, \eta_h \in B_h, \tag{6.10}$$

for any $\phi_h \in \widetilde{\mathcal{A}}_h$. In our case, because of (2.12), the problem is self-adjoint and $\bar{\boldsymbol{p}}_h = \bar{\boldsymbol{u}}_h$.

We now apply our results from Section 5.4 to compute (6.10). However, our formulas only consider bulk functionals (not boundary functionals). Thus, we restrict our problem by taking $\gamma_{\mathrm{N}} = 0$, $\Gamma_{\mathrm{D}} = \emptyset$, and $\boldsymbol{g}_{\mathrm{N}} \neq \mathbf{0}$ only within $\Sigma \subset \partial\widehat{\mathfrak{D}}$. This allows us to avoid differentiating any boundary integrals. In addition, for convenience, we take $\boldsymbol{f} = \mathbf{0}$, which implies that $\chi_h(\Omega_h; \boldsymbol{v}_h)$ is independent of any shape perturbations in $\mathcal{C}(\Sigma)$.

Evaluating the Fréchet derivatives, we obtain for all $\phi_h \in \widetilde{\mathcal{A}}_h$ that

$$\chi_h' \left(\Omega_h(\phi_h); \boldsymbol{v}_h\right)(\eta_h) = 0, \quad J'\left(\Omega_h(\phi_h); \boldsymbol{v}_h\right)(\eta_h) = -a_0 \int_{\Gamma_h(\phi_h)} \frac{\eta_h}{|\nabla \phi_h|} dS(\boldsymbol{x}),$$

$$A_h'\left(\Omega_h(\phi_h); \boldsymbol{u}_h, \boldsymbol{v}_h\right)(\eta_h) = -\int_{\Gamma_h(\phi_h)} \left(2\mu \boldsymbol{\varepsilon}(\nabla \boldsymbol{u}_h) : \boldsymbol{\varepsilon}(\nabla \boldsymbol{v}_h) + \lambda(\nabla \cdot \boldsymbol{u}_h)(\nabla \cdot \boldsymbol{v}_h)\right) \frac{\eta_h}{|\nabla \phi_h|} dS(\boldsymbol{x}), \tag{6.11}$$

for all $\boldsymbol{u}_h, \boldsymbol{v}_h \in V_h(\Omega_h(\phi_h))$, and all $\eta_h \in B_h$, where a_0 is the penalty parameter in (2.12). Note that the facet stabilization terms in (3.19) do not contribute anything because we take the facet patch selections to be fixed and independent of the perturbation η_h. Hence, since $\bar{\boldsymbol{p}}_h = \bar{\boldsymbol{u}}_h$, (6.10) reduces to

$$\begin{aligned} \mathcal{J}'\left(\phi_h\right)(\eta_h) &= L'\left(\phi_h; \bar{\boldsymbol{u}}_h(\phi_h), \bar{\boldsymbol{p}}_h(\phi_h)\right)(\eta_h) \\ &= \int_{\Gamma_h(\phi_h)} \left(2\mu |\boldsymbol{\varepsilon}(\nabla \bar{\boldsymbol{u}}_h)|^2 + \lambda(\nabla \cdot \bar{\boldsymbol{u}}_h)^2 - a_0\right) \frac{\eta_h}{|\nabla \phi_h|} dS(\boldsymbol{x}). \end{aligned} \tag{6.12}$$

Implementing (6.12) is straightforward within an unfitted finite element software, e.g. `ngsolve` [67], `ngsxfem` [49], provided Assumption 4 holds. Otherwise, we need to compute (5.74), which can be tedious. Fortunately, since ϕ_h is a piecewise polynomial, the set E in (5.74) must equal the entire facet F, which delivers some simplification. But (5.74) is still non-linear in the perturbation η_h. In our computations, we simply choose a side of F, either T_+ or T_-, which is automatically done by `ngsxfem` because the domain boundary is never allowed to fall exactly on a mesh facet.

6.4. Shape Optimization Algorithm

Our algorithm is essentially gradient descent. Let $B(\omega_h, \eta_h)$ be a bilinear form defined for all ω_h, η_h in B_h; for example, we may take $B(\omega_h, \eta_h) = (\omega_h, \eta_h)_{H^1(\widehat{\mathfrak{D}})}$. Moreover, we introduce the following restricted finite element space $Q_h = \{\varphi_h \in B_h : \varphi_h|_\Sigma = 0\}$.

Then, given a current domain $\Omega_h(\phi_h)$, we find a descent direction $\delta\phi_h \in Q_h$ that satisfies

$$B\left(\delta\phi_h, \eta_h\right) = -\mathcal{J}'\left(\phi_h\right)\left(\eta_h\right), \quad \forall\, \eta_h \in Q_h. \tag{6.13}$$

We then update ϕ_h by $\phi_h \leftarrow \phi_h + \alpha\delta\phi_h$, where $\alpha > 0$ is a step-size determined through a back-tracking line search. Note that the choice of the facet patches for stabilization stays fixed during the line search.

As mentioned earlier in Section 6.1, we want the level set function ϕ_h to satisfy $|\nabla\phi_h| \approx 1$ or at least $|\nabla\phi_h| \geq \frac{1}{2}$. To satisfy this requirement, we start with an initial level set function which is the signed distance function for our initial shape, hence $|\nabla\phi_h| = 1$ almost everywhere. The shape optimization algorithm however does not preserve this property and over many iterations we may no longer have $|\nabla\phi_h| \approx 1$. To remedy this, we reinitialize ϕ_h to that of a signed distance function after a set number of iterations.

Several methods for level set reinitialization on unstructured grids exist, such as the DRLSE algorithm [51], in which the reinitialization involves solving a fully explicit difference scheme. Other methods include [59], which use local projections and [3], which uses a fixed-point method.

In our algorithm, we compute the signed distance function directly by over sampling the boundary, computing the signed distance to the boundary from every node on the mesh, and then interpolating to a function in the background finite element space. One can also use the method in [65].

Chapter 7. Numerical Results for Shape Optimization

We include some numerical experiments of the full PDE minimization problem as well as some numerical tests to confirm the validity of the shape derivative formulation.

In each of the following simulations we use a level set formulation, with a fixed background mesh, to define the boundary of Ω. We start by checking the validity of our shape derivative formula in the elasticity PDE framework by performing two tests using a finite difference approximation of the shape derivative.

7.1. Shape Derivative Test

First, we fixed an initial shape, and then compare our shape derivative formula with an increasingly better finite difference approximation. I.e., we approximate the shape derivative by

$$J'_{\mathrm{FD}}(\phi_h)(\eta_h) = \frac{J(\phi_h + \epsilon\eta_h) - J(\phi_h)}{\epsilon},$$

and then compare J'_{FD} to our shape derivative formula for decreasing ϵ. The exact shape derivative $J'_{\mathrm{exact}}(\phi_h)(\eta_h)$ is given by (6.12).

We use degree $k = 1$ for B_h and set $\phi_h = I_h\phi$ and $\eta_h = I_h\eta$, where I_h is the standard nodal interpolant for B_h. In doing the comparison, we compute the following

$$\zeta(\epsilon) = \frac{|J'_{\mathrm{exact}} - J'_{\mathrm{FD}}|}{\epsilon}.$$

For this simulation, we fix the design domain $\widehat{\mathfrak{D}} := (0.0, 2.0) \times (0.0, 1.0)$ and choose the initial shape (Figure 7.1) $\Omega := \widehat{\mathfrak{D}} \setminus B_r(\boldsymbol{x}_0)$, where $r = 0.2$ and $\boldsymbol{x}_0 = (0.3, 0.3)$ and $B_r(\boldsymbol{x}_0)$ is the ball of radius r centered at $\boldsymbol{x}_0$. We use a continuous piecewise linear finite element space and choose an arbitrary direction to compute the shape derivative, and then

(a) Initial shape

(b) Perturbed shape

Figure 7.1. We have an example of an initial shape and an arbitrary perturbation of that shape.

compare our shape derivative formula (6.12) to an increasingly better finite difference approximation of the shape derivative.

Here are the results:

Table 7.1. Shape Derivative Test

eps	$J(\phi_h)$	$J(\phi_h + \epsilon\eta_h)$	J'_{exact}	J'_{FD}	$\lvert J'_{\text{exact}} - J'_{\text{FD}}\rvert$	$\zeta(\epsilon)$
1.00E-01	0.75860	0.95387	0.38283	1.95275	1.56992e+00	15.69922
1.00E-02	0.75860	0.76296	0.38283	0.43641	5.35852e-02	5.35852
1.00E-03	0.75860	0.75899	0.38283	0.38804	5.21949e-03	5.21949
1.00E-04	0.75860	0.75864	0.38283	0.38332	4.93417e-04	4.93417
1.00E-05	0.75860	0.75860	0.38283	0.38287	4.94585e-05	4.94585
1.00E-06	0.75860	0.75860	0.38283	0.38283	4.90236e-06	4.90236
1.00E-07	0.75860	0.75860	0.38283	0.38283	6.47544e-07	6.47544
1.00E-08	0.75860	0.75860	0.38283	0.38283	3.88828e-06	388.82848

The last entry in Table 7.1 is expected due to the roundoff and truncation error from the finite difference approximation for small ϵ.

7.2. Shape Derivative Translation Test

Second, we test the formula by choosing different initial shapes and computing the shape derivative in arbitrary directions. In practice, we chose a shape consisting of the entire design domain $\widehat{\mathfrak{D}}$ minus a hole and then translate the hole to get different inital shapes.

For this simulation, we fix $\epsilon = 1.00E{-}07$ and choose initial shape like that depicted in Figure 7.1 for the first iteration ($\Omega := \widehat{\mathfrak{D}} \setminus B_r(\boldsymbol{x}_0)$, where $r = 0.2$ and $\boldsymbol{x}_0 = (0.3, 0.3)$ and $B_r(\boldsymbol{x}_0)$ is the ball of radius r centered at $\boldsymbol{x}_0$) and compare it with J'_{FD}. Then for subsequent iterations, we translate the hole by $\boldsymbol{v} = (0.1, 0.05)$ after every iteration. We use a continuous piecewise linear finite elements for every iteration.

Table 7.2. Shape Derivative Translation Test

it	$J(\phi_h(\cdot,t))$	$J(\phi_h(\cdot,t)+\epsilon\eta_h(\cdot))$	J'_{exact}	J'_{FD}	$\lvert J'_{\text{exact}} - J'_{\text{FD}}\rvert$	ζ
0	0.75860	0.75860	0.38283	0.38283	6.47544e-07	6.47544
1	0.74186	0.74186	0.13959	0.13959	1.25195e-06	12.51948
2	0.73253	0.73253	0.03503	0.03503	3.21555e-07	3.21555
3	0.72807	0.72807	0.02159	0.02159	4.34587e-07	4.34587
4	0.72670	0.72670	0.05205	0.05205	3.60208e-09	0.03602
5	0.72722	0.72722	0.08675	0.08675	8.78340e-08	0.87834
6	0.72883	0.72883	0.10066	0.10066	2.01567e-08	0.20157
7	0.73113	0.73113	0.08418	0.08418	4.94938e-07	4.94938

7.3. Simple Example

This is a simple geometric shape optimization problem for testing purposes. Let $u = u(x, y)$ be a given function defined by

$$\begin{aligned} u(x,y) &= \frac{1}{p}\left(\frac{1}{\alpha}x^p + \frac{1}{\beta}y^p\right), \\ \nabla u &= \left(\frac{1}{\alpha}x^{p-1}, \frac{1}{\beta}y^{p-1}\right) \quad \Rightarrow \quad |\nabla u|^2 = \left(\frac{x^{p-1}}{\alpha}\right)^2 + \left(\frac{y^{p-1}}{\beta}\right)^2, \end{aligned} \tag{7.1}$$

given $\alpha, \beta > 0$. Next, let $\lambda > 0$ and $A_0 > 0$ be given, and define the following shape functional:

$$J(\Omega) = \int_\Omega |\nabla u|^2 \, dA - \lambda \left(|\Omega| - A_0\right), \tag{7.2}$$

and note that u does not depend on Ω. Applying standard shape differentiation formulas, we get

$$\delta J(\Omega; \boldsymbol{V}) = \int_{\partial\Omega} \left(|\nabla u|^2 - \lambda\right) \boldsymbol{V} \cdot \boldsymbol{\nu} dS, \tag{7.3}$$

for all smooth $\boldsymbol{V}$. For any critical point Ω^* of (7.2), we must have $\delta J(\Omega^*; \boldsymbol{V}) = 0$ for all smooth $\boldsymbol{V}$, which means the integrand must vanish. In other words,

$$\begin{aligned} &|\nabla u|^2 = \lambda, \quad \text{for all } (x, y) \in \partial\Omega^*, \\ \Rightarrow \quad &\left(\frac{x^{p-1}}{\alpha\sqrt{\lambda}}\right)^2 + \left(\frac{y^{p-1}}{\beta\sqrt{\lambda}}\right)^2 = 1, \end{aligned} \tag{7.4}$$

which is the equation for a superellipse, i.e. $\partial\Omega^*$ is a superellipse. If we take A_0 to be the desired area of the superellipse, then we must have

$$4(\alpha\beta\lambda)^{\frac{1}{p-1}} \frac{\left(\Gamma\left(1 + \frac{1}{2p-2}\right)\right)^2}{\Gamma\left(1 + \frac{1}{p-1}\right)} = A_0, \tag{7.5}$$

where Γ represents the Gamma function, and so λ is uniquely determined by A_0.

In our numerical test, we take $\alpha = 1$, $\beta = 2$, $\lambda = 0.18$, and $p = 4$. The design domain is $\widehat{\mathfrak{D}} := (-1.0, 1.0) \times (-1.1, 1.1)$ and the initial guess for the optimal shape is a disk of radius 0.5 centered at the origin. We use $k = 1, 2, 3$ for B_h in the level set approximation of ϕ_h. The stopping criteria for each simulation was when the difference in J between successive iterations was less than 10^{-8}. See Table 7.3 for a list of converged J and J' values for different mesh sizes. The computed values of J' are the vector 2-norm of the coefficients of the basis representation of the linear form: $J'(\phi_h)(\eta_h) = ((|\nabla u|^2 - \lambda)|\nabla\phi_h|^{-1}, \eta_h)_{\partial\Omega_h(\phi_h)}$. Since $p = 4$, the superellipse can be represented *exactly* by a discrete level set function using degree 6 piecewise polynomials. Thus, we computed the exact value of the cost at the minimizer, which is $J_{\text{exact}} = -0.3702425373188486$ and we confirmed that $|J'_{\text{exact}}| = 3.3 \cdot 10^{-18}$.

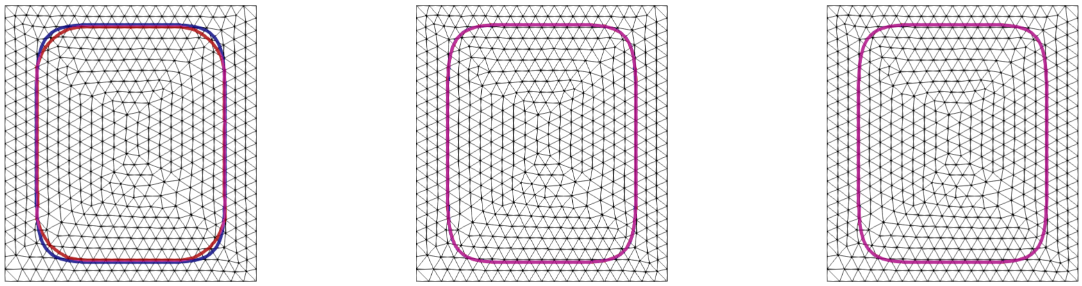
The `ngsxfem` add-on package to NGSolve uses an isoparametric mapping for implementing higher order unfitted schemes. But this is technically outside of our theory because we assume exact integration on the higher order interface without invoking an isoparametric map. On the other hand, `ngsxfem` provides an alternative method for integrating with higher order interfaces that uses subdivision of the underlying mesh. Essentially, with enough subdivision levels, one can get a sufficiently accurate approximation of the various integrals, which is the approach we use in this superellipse experiment.

Table 7.3. Ellipse Shape Derivative Test

maxh	$k=1$		$k=2$		$k=3$	
	$\lvert J - J_{\text{exact}}\rvert$	$\lvert J'\rvert$	$\lvert J - J_{\text{exact}}\rvert$	$\lvert J'\rvert$	$\lvert J - J_{\text{exact}}\rvert$	$\lvert J'\rvert$
0.1	1.1700e-03	1.7223e-02	3.6038e-05	1.5115e-06	1.9625e-07	9.0576e-08
0.05	7.3293e-04	5.0726e-03	4.8018e-06	3.7531e-07	9.5482e-09	4.3523e-08
0.025	1.7098e-04	2.2085e-03	2.0907e-07	1.2123e-07	1.9605e-10	1.6617e-08
0.0125	5.7855e-05	7.8292e-04	9.4514e-08	7.6382e-08	5.7451e-11	1.5158e-08

Figure 7.2 shows plots of the numerical minimizers compared against the exact minimizer. We now discuss the practical issue of when the discrete boundary, $\partial\Omega_h$, lies along a mesh facet (recall Section 5.5). First, note that if $\partial\Omega_h$ has a non-trivial intersection with a facet F, then it must lie along the *entire* facet, because $\partial\Omega_h$ is represented by piecewise polynomials. Moreover, the `ngsxfem` package avoids these ambiguous situations by adding a small number, e.g. 10^{-14}, to the nodal values of the level set function ϕ_h that lie along the facet. In effect, this forces the derivative formula (5.74) to "choose a side."

Nevertheless, when the boundary does lie along a facet, the derivative of the cost is discontinuous at that facet. The practical effect on the optimization is that the numerical interface, $\partial\Omega_h$, can be "faceted." In Figure 7.2(a), aside from the rounded corners where the numerical minimizer (red) deviates from the exact minimizer (blue), we see that the



(a) Polynomial degree $k = 1$ (b) Polynomial degree $k = 2$ (c) Polynomial degree $k = 3$

Figure 7.2. The exact interface is in blue, the approximate interface is in red.

red interface (mostly) follows the mesh facets along the nearly straight portions of the interface. The exact interface, for the most part, does *not* lie along any mesh facets. This is particularly noticeable at the bottom left of Figure 7.2(a)

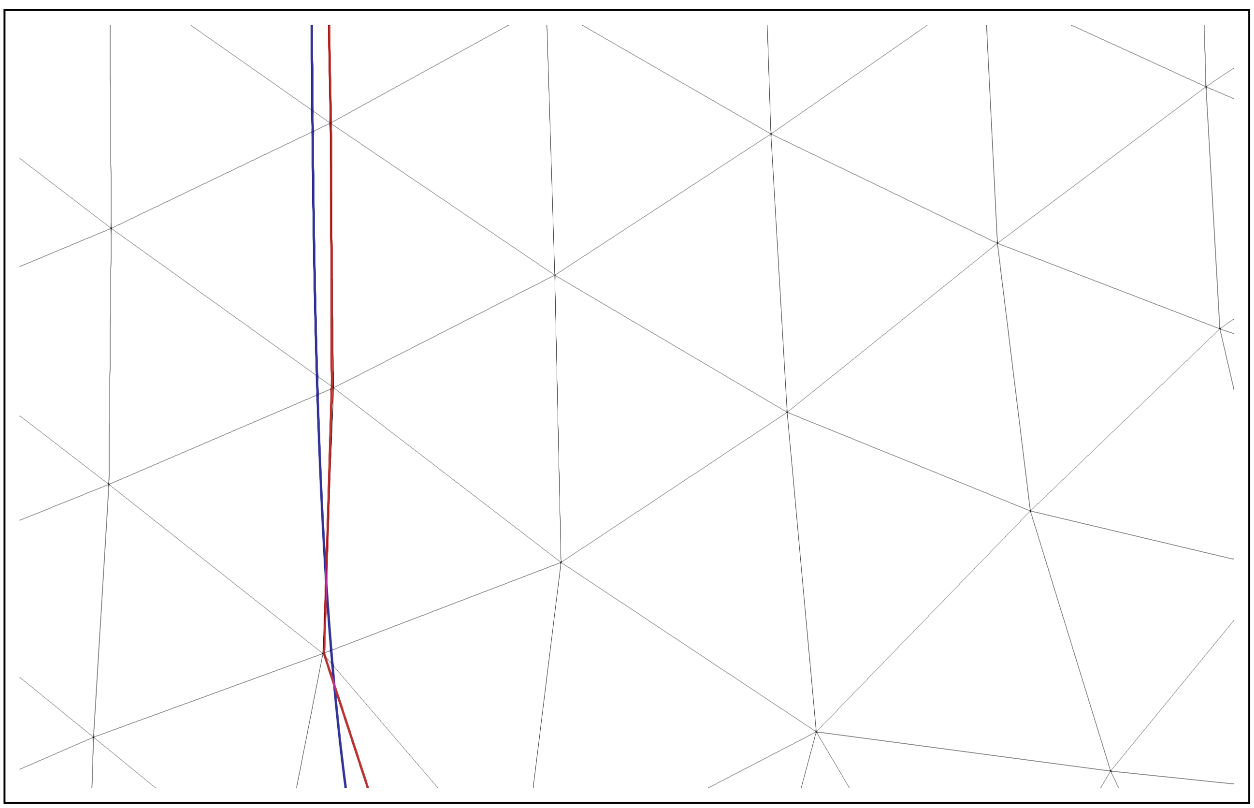


Figure 7.3. Expanded view of Figure 7.2 (a).

It is not surprising that the exact discrete minimizer has some mesh dependence. In these experiments, and others we have run, this effect is fairly mild. Moreover, this faceting effect is significantly reduced when using higher order methods, as Figure 7.2(b,c) indicates.

7.4. Shape Optimization Elasticity

We introduce a numerical simulation of the PDE constrained minimization problem (2.4), with the compliance shape functional (2.12)

$$J(\Omega; \boldsymbol{v}) = \chi(\Omega; \boldsymbol{v}) + a_0|\Omega|,$$

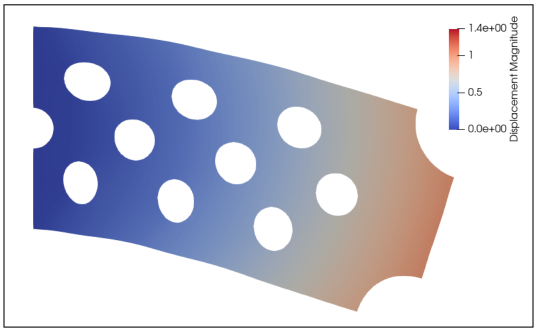
In this instance, the area penalization parameter is $a_0 = 0.3$ and we choose material parameters $\lambda = 0$ $\mu = 5$ in the linear elasticity PDE. Additionally, we choose facet stabilization parameter $\gamma_{\mathrm{s}} = 2$ with layer thickness parameter $\delta = h$, and choose Nitsche stabilization parameters $\gamma_{\mathrm{D}} = 10\mu$ and $\gamma_{\mathrm{N}} = 0$.

Figure 7.4. Left: Initial shape. Right: level set function constraint set $\Sigma \subset \widehat{\mathfrak{D}}$.

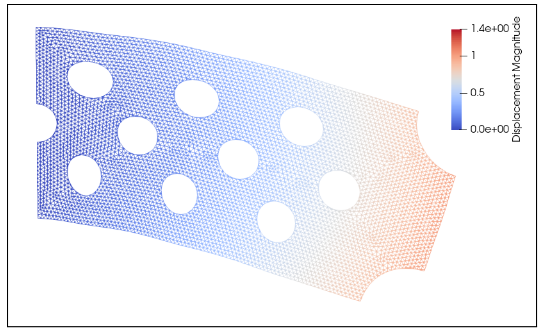
We mimic the setup of [17] in order to corroborate our results. We choose the initial shape as depicted in Figure 7.4 (left). We define the design domain to be $\widehat{\mathfrak{D}} := (0.0, 2.0) \times (0.0, 1.0)$ and choose an initial shape of $\widehat{\mathfrak{D}}$ with 12 holes: 10 of which have radius 0.1 and are evenly spaced, and the remaining two are centered at the top right and bottom right corners having radius 0.25. Additionally, $\widehat{\Gamma}_{\mathrm{D}} = \emptyset$ as we previously assumed and Γ_D consists of the line segment between $(0.0, 0.0)$ and $(0.0, 0.15)$ and a second line segment between $(0.0, 1.0)$ and $(0.0, 0.85)$. Also, $\boldsymbol{g}_N = (0.0, -1.0)$ on the line segment between $(2.0, 0.4)$ and $(2.0, 0.6)$ (i.e. on Γ_N).

Note that the level set function is constrained to *not* change along $\Sigma \subset \partial\widehat{\mathfrak{D}}$ as depicted in Figure 7.4 (right). This is to ensure the feasibility of the resulting shape.

Here are some of the results:

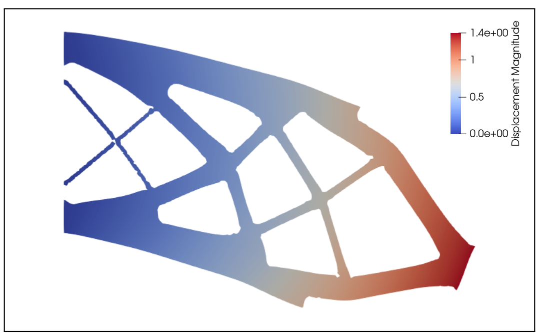


(a) The initial guess and an exaggerated displacement of the cantilever is shown

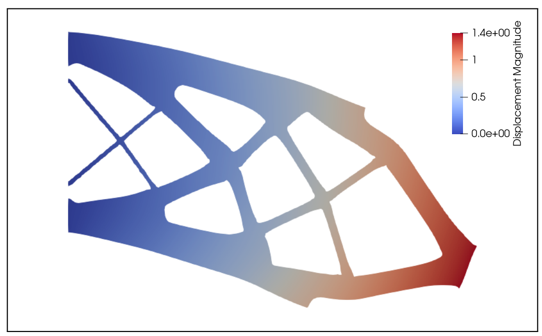


(b) We have the same initial shape as above now with the mesh being shown.

Figure 7.5. Initial shape



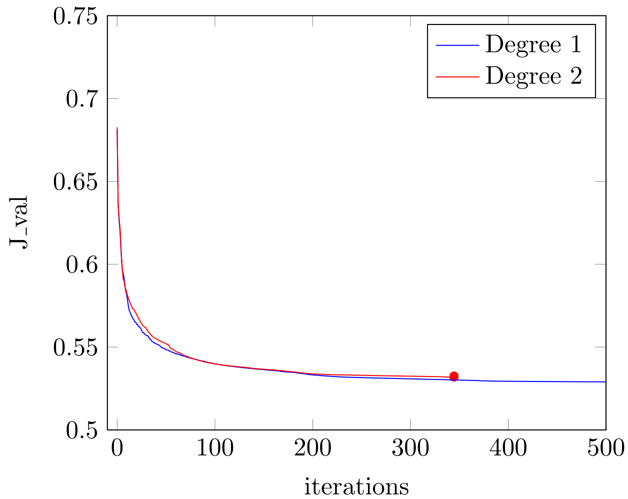
(a) Piecewise linear finite elements with an exaggerated displacement.



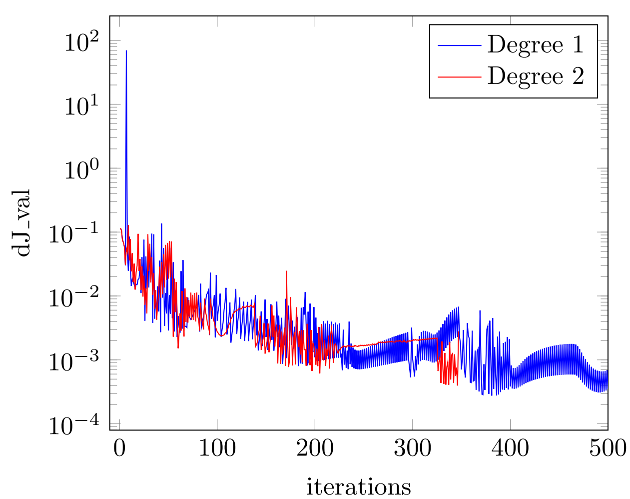
(b) Piecewise quadratic finite elements with an exaggerated displacement.

Figure 7.6. Resulting shapes for piecewise linear and quadratic finite elements

The resulting optimal shapes for both piecewise linear and piecewise quadratic B_h are nearly identical (see Figure 7.6). The optimization history is given in Figure 7.7. The optimization for degree $k = 2$ used the isoparametric mapping approach in `ngsxfem` because the subdivision method would have been prohibitively expensive. Since the mesh size was $h = 0.02$, the isoparametric mapping was only a small perturbation from a linear triangle element. Nevertheless, this does induce a small error in our shape derivative, which introduces a small error when computing a descent direction. This is evidenced by the red curve in Figure 7.7(a) stopping at iteration index ≈ 340.



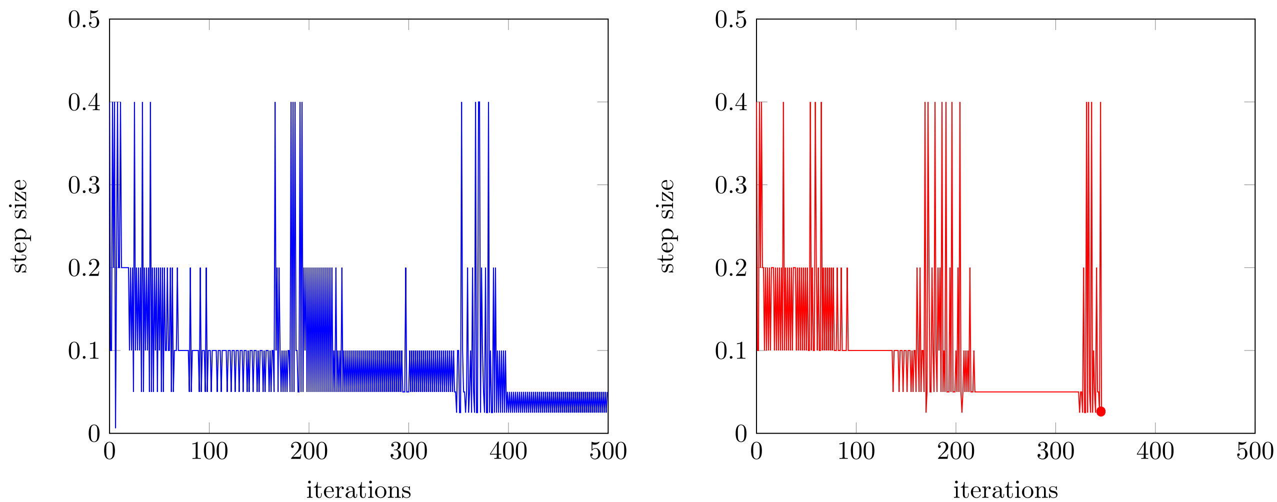
(a) Cost vs. iteration number for piecewise linear (blue) and piecewise quadratic (red) finite element methods.



(b) Norm of δJ vs. iteration number for piecewise linear (blue) and piecewise quadratic (red) finite element methods.

Figure 7.7. Cost and Norm of δJ vs. iteration number

We also plot the step size vs iteration number in Figure 7.8.



(a) Piecewise linear finite elements

(b) Piecewise quadratic finite elements

Figure 7.8. Step size vs. iteration number

Chapter 8. Remarks on Unfitted Shape Optimization

We presented a numerical shape optimization technique that takes advantage of unfitted finite element methods. We showed how to compute the exact discrete shape derivative of bulk shape functionals, under mild assumptions, and established the Fréchet differentiability of discrete bulk shape functionals. This is done using both the perturbation of the identity approach, as well as direct perturbation of the level set representation of the domain. Our formulation allows for including a discrete PDE constraint and our discrete derivative mimics the shape derivative formula from the continuous problem. In other words, our method enjoys advantages of both the discretize-then-optimize and optimize-then-discretize philosophies.

We illustrated our method by considering the shape optimization of an elastic body. Specifically, we used a Lagrangian approach to deal with the linear elasticity PDE constraint. Furthermore, our level set based shape derivative approach allowed for *directly* optimizing the level set representation of the domain. No ad-hoc extension velocities were needed to update the level set function. Our numerical results demonstrated the effectiveness of our approach. For instance, the step sizes chosen by our gradient descent method are not excessively small, which can happen with some optimize-then-discretize approaches.

Our method can be easily applied to a two-phase material problem, such as an elastic body with a fixed shape but with two different material regions, Ω_1 and Ω_2, inside. In this case, the level set function marks one of the phases, say Ω_1, and the weak formulation involves a sum over the two sub-domains. As long as there is no boundary integral over $\partial\Omega_1 \cap \partial\Omega_2$ in the weak form, our methodology can be applied.

A point of future work is to extend our method to handle boundary functionals. Most likely, this will require some kind of regularization of the cost functional. Another area to investigate is the connection of our method to time-dependent problems, i.e. to extend our approach to solving PDEs in time-dependent geometries, as well as shape optimization with time-varying shape constraints.

Chapter 9. Landau–de Gennes Model

Modeling liquid crystals in three dimensions at the continuum level involves the use of a tensor order parameter Q that is symmetric and traceless, i.e. it belongs to

$$\mathbf{S}_0 := \{Q \in \mathbb{R}^{3\times 3} \mid Q^{\mathsf{T}} = Q,\ \mathrm{tr}(Q) = 0\}. \tag{9.1}$$

Since Q is based on a probability distribution of LC molecules, the eigenvalues of Q, denoted λ_i, satisfy

$$-\frac{1}{3} \leq \lambda_i(Q) \leq \frac{2}{3}, \quad \text{for } i = 1, 2, 3, \tag{9.2}$$

and, since Q is traceless, $\lambda_3 = -(\lambda_1 + \lambda_2)$. When all eigenvalues are equal, then they are 0 and $Q = 0$, which represents the isotropic state. If all eigenvalues are distinct, then Q is in a *biaxial* state. However, usually Q has a single largest eigenvalue with the other two eigenvalues equal; this is called a *uniaxial* state and Q may be expressed as

$$Q = s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I\right), \tag{9.3}$$

where $\mathbf{n}$, which has unit length $|\mathbf{n}| = 1$, is the eigenvector of the largest eigenvalue. The scalar order parameter s is called the *degree-of-orientation* and is a measure of the orientational order of the LC molecules, and $\mathbf{n}$ is called the *director* that represents the average direction in which the molecules are pointing. Note that $-\frac{1}{2} \leq s \leq 1$.

For LCs in a physical domain Ω, we model the LC state through a tensor-valued function $Q : \Omega \to \mathbf{S}_0$. We assume Ω has Lipschitz boundary Γ with outward pointing unit normal vector $\boldsymbol{\nu}$. The free energy of the LdG model is defined as [55, 56, 64]:

$$\begin{aligned}\mathcal{E}[Q] := &\int_\Omega f(Q, \nabla Q)\, d\mathbf{x} + \int_\Omega \psi(Q)\, d\mathbf{x} \\ &+ \int_\Gamma g(Q)\, dS(\mathbf{x}) + \int_\Gamma \phi(Q)\, dS(\mathbf{x}) - \int_\Omega \chi(Q)\, d\mathbf{x},\end{aligned} \tag{9.4}$$

with the elastic energy (with twist component as in [73, 64]) given by

$$f(Q,\nabla Q) := \frac{1}{2}\Big(\ell_1|\nabla Q|^2 + \ell_2|\nabla\cdot Q|^2 + \ell_3(\nabla Q)^{\mathsf{T}} \vdots \nabla Q \\ + 4\ell_1\tau_0\nabla Q \vdots (\varepsilon\cdot Q)\Big), \tag{9.5}$$

where $\{\ell_i\}_{i=1}^3$ (units of $\mathrm{J}\cdot\mathrm{m}^{-1}$) and τ_0 (units of m^{-1}) are material dependent elastic constants, and ψ is a "bulk" potential, ε is the Levi-Civita symbol, and

$$|\nabla Q|^2 := Q_{ij,k}Q_{ij,k}, \quad |\nabla\cdot Q|^2 := Q_{ij,j}Q_{ik,k}, \\ (\nabla Q)^{\mathsf{T}} \vdots \nabla Q := Q_{ij,k}Q_{ik,j}, \quad \nabla Q \vdots (\varepsilon\cdot Q) := \varepsilon_{jkl}Q_{ik,l}Q_{ij}, \tag{9.6}$$

where we use the convention of summation over repeated indices and ε_{jkl} is the Levi–Civita tensor. The transpose in the third term indicates to swap one of the Q indices with the derivative index. The elastic constants in the LdG model can be related to the elastic constants in the Oseen–Frank model (see [55, 56]). Note that taking $\ell_i = 0$, for $i = 2, 3$, and $\tau_0 = 0$ gives the often used one constant LdG model. More complicated models can also be considered [56, 31, 70].

Next, the bulk potential ψ is a double-well type of function that is given by

$$\psi(Q) = a_0 - \frac{a_2}{2}\mathrm{tr}(Q^2) - \frac{a_3}{3}\mathrm{tr}(Q^3) + \frac{a_4}{4}\Big(\mathrm{tr}(Q^2)\Big)^2. \tag{9.7}$$

Above, a_2, a_3, a_4 are material parameters (units of $\mathrm{J}\cdot\mathrm{m}^{-3}$) such that a_2, a_3, a_4 are positive; a_0 is a convenient constant to ensure $\psi \geq 0$. Stationary points of ψ are either uniaxial or isotropic Q-tensors [52].

The surface energy, composed of the quadratic $g(Q)$ and higher-order boundary potential $\phi(Q)$, accounts for *weak anchoring* of the LC (i.e. penalization of boundary conditions). For example, a Rapini-Papoular type anchoring energy [2] can be considered:

$$g(Q) = \frac{w_0}{2}|Q - Q_\Gamma|^2 + \frac{w_1}{2}|\tilde{Q} - \tilde{Q}^\perp|^2, \quad \tilde{\phi}(Q) = \frac{w_2}{4}\big(|\tilde{Q}|^2 - s_0^2\big)^2, \tag{9.8}$$

where w_0, w_1, and w_2 are positive constants (units of $\mathrm{J} \cdot \mathrm{m}^{-2}$), $Q_\Gamma(x) \in \mathbf{S}_0$ for all $\mathbf{x} \in \Gamma$, and s_0 is the scalar order parameter of the uniaxial Q that minimizes the double well. We set $\tilde{Q} := Q + \frac{s_0}{3} I$, and define the standard projection onto the plane orthogonal to $\boldsymbol{\nu}$, that is, $Q^\perp := \Pi Q \Pi$ where $\Pi = I - \boldsymbol{\nu} \otimes \boldsymbol{\nu}$. We define Q_Γ to be uniaxial of the form

$$Q_\Gamma = s_0 \left(\boldsymbol{\nu} \otimes \boldsymbol{\nu} - \frac{1}{3} I \right). \tag{9.9}$$

The w_0 term in (9.8) models homeotropic (normal) anchoring, while w_1 and w_2 model planar degenerate anchoring.

For the analysis, we modify the "boundary" potential to have quadratic growth. Let $\rho : [0, \infty) \to \mathbb{R}_+$ be a smooth cut-off function, i.e.

$$\begin{cases} \rho(r) = 1 & \text{if } r < b_1, \\ \rho(r) = \text{ monotone} & \text{if } b_1 \le r \le b_2, \\ \rho(r) = 0 & \text{if } r > b_2, \end{cases}$$

where $1 \le b_1 < b_2$ are fixed constants. We then modify the boundary potential

$$\phi(Q) = \tilde{\phi}(Q) \rho(|Q|^2) + w_2^2 |Q|^2 \left(1 - \rho(|Q|^2) \right), \tag{9.10}$$

which then implies the following estimates

$$|\phi(Q)| \le \frac{w_2 s_0^4}{4} + c_0 |Q|^2, \qquad |\phi'(Q)| \le c_1 |Q|, \qquad |\phi''(Q)| \le c_2. \tag{9.11}$$

Where c_0, c_1, and c_2 are constant.

The function $\chi(\cdot)$ models external forcing on the LC system. Usually, $\chi(Q)$ is taken to be linear in Q, i.e. $\chi(Q) = U_\Omega : Q$, where $U_\Omega : \Omega \to \mathbb{R}^{3 \times 3}$ is a given function. For instance, the energy density of a dielectric LC with fixed boundary potential is given by

$-1/2\,\mathbf{D}\cdot\mathbf{E}$ [75], where the electric displacement $\mathbf{D}$ is related to the electric field $\mathbf{E}$ by the linear constitutive law [27, 31, 10]:

$$\mathbf{D} = \boldsymbol{\varepsilon}\mathbf{E} = \bar{\varepsilon}\mathbf{E} + \varepsilon_{\mathrm{a}} Q\mathbf{E}, \quad \boldsymbol{\varepsilon}(Q) = \bar{\varepsilon} I + \varepsilon_{\mathrm{a}} Q, \tag{9.12}$$

where $\boldsymbol{\varepsilon}$ is the LC material's dielectric tensor and $\bar{\varepsilon}$, ε_{a} are constitutive dielectric permittivities. Thus, we may rewrite the dielectric energy density as

$$-\frac{1}{2}\mathbf{D}\cdot\mathbf{E} = -\frac{1}{2}\bar{\varepsilon}|\mathbf{E}|^2 + \chi(Q), \quad \chi(Q) = -\frac{1}{2}\varepsilon_{\mathrm{a}}\mathbf{E}\cdot Q\mathbf{E} \equiv -\frac{1}{2}\varepsilon_{\mathrm{a}}\mathbf{E}\otimes\mathbf{E} : Q = U_\Omega : Q, \tag{9.13}$$

where $\chi(Q)$ has units of J/m^3 and $U_\Omega = -(1/2)\varepsilon_{\mathrm{a}}\mathbf{E}\otimes\mathbf{E}$. We do not include the term $(\bar{\varepsilon}/2)|\mathbf{E}|^2$ in (9.4) because it is independent of Q.

9.1. Basic Theory

The function space for posing the weak formulation of the time-dependent LdG problem is given by $\mathbf{Q} := H^1(\Omega;\mathbf{S}_0)$. Note that $\mathbf{S}_0$ can be uniquely identified with a five dimensional vector space [30], i.e. there exists 3×3, symmetric traceless basis matrices $\{E^i\}_{i=1}^5$ such that any $Q\in\mathbf{S}_0$ can be uniquely expressed as $Q = q_i E^i$, for some coefficients $q_1,\ldots,q_5$. Therefore, $\mathbf{Q}$ is isomorphic to $H^1(\Omega;\mathbb{R}^5)$.

We now summarize some basic results that are needed in the well-posedness of the weak formulation. The following theorem [21, Lem. 4.1] establishes this result for the ℓ_1, ℓ_2, ℓ_3 terms in the elastic energy.

Theorem 9.1. *Let $a_e(\cdot,\cdot) : \mathbf{Q}\times\mathbf{Q}\to\mathbb{R}$ be the symmetric bilinear form defined by*

$$a_e(Q,P) := \ell_1 (Q_{ij,k}, P_{ij,k})_\Omega + \ell_2 (Q_{ij,j}, P_{ik,k})_\Omega + \ell_3 (Q_{ij,k}, P_{ik,j})_\Omega . \tag{9.14}$$

Then $a_e(\cdot,\cdot)$ is bounded. If ℓ_1, ℓ_2, ℓ_3 satisfy

$$0 < \ell_1, \quad -\ell_1 < \ell_3 < 2\ell_1, \quad -\frac{3}{5}\ell_1 - \frac{1}{10}\ell_3 < \ell_2, \tag{9.15}$$

then there is a constant $c > 0$ *such that* $a_e(P,P) \geq c\|\nabla P\|_{0,\Omega}^2$ *for all* $P \in \mathbf{Q}$.

Proposition 9.2 (Coercivity)**.** *Let* $s(\cdot,\cdot) : \mathbf{Q} \times \mathbf{Q} \to \mathbb{R}$ *be the symmetric bilinear form defined by*

$$s(Q,P) = w_0(Q,P)_\Gamma + w_1\left(Q - Q^\perp, P\right)_\Gamma. \tag{9.16}$$

There exists a constant $\alpha_1 > 0$ *such that*

$$a_e(P,P) + s(P,P) \geq \alpha_1\|P\|_{1,\Omega}^2, \qquad \forall P \in \mathbf{Q}. \tag{9.17}$$

We also have the bilinear form $a_{\mathrm{t}}(\cdot,\cdot) : \mathbf{Q} \times \mathbf{Q} \to \mathbb{R}$, which is *not* coercive, accounting for the twist term:

$$a_{\mathrm{t}}(Q,P) := 2\ell_1\tau_0\left[\varepsilon_{ikl}(Q_{jk,l},P_{ij})_\Omega + \varepsilon_{ikl}(P_{jk,l},Q_{ij})_\Omega\right], \tag{9.18}$$

and satisfies the bound

$$a_{\mathrm{t}}(Q,P) \leq 2\ell_1\tau_0\sqrt{27}\left[|Q|_{1,\Omega}\|P\|_{0,\Omega} + |P|_{1,\Omega}\|Q\|_{0,\Omega}\right]. \tag{9.19}$$

For later use, we define one bilinear form to contain (9.14), (9.16), and (9.18):

$$b^i(Q,P) = a_{\mathrm{e}}(Q,P) + a_{\mathrm{t}}(Q,P) + s(Q,P), \tag{9.20}$$

which satisfies the following continuity result.

Proposition 9.3 (Continuity)**.** *There holds*

$$\begin{aligned} a_e(Q,P) \leq c_e|Q|_{1,\Omega}|P|_{1,\Omega}, \quad a_t(Q,P) \leq c_t\|Q\|_{1,\Omega}\|P\|_{1,\Omega}, \\ s(Q,P) \leq c_s\|Q\|_{0,\Gamma}\|P\|_{0,\Gamma}, \quad b^i(Q,P) \leq c_0\|Q\|_{1,\Omega}\|P\|_{1,\Omega}, \end{aligned} \tag{9.21}$$

for all $Q, P \in \mathbf{Q}$*, where*

$$c_e = \ell_1 + 3\ell_2 + \ell_3,\; c_t = 2\sqrt{27}\ell_1\tau_0,\; c_s = w_0 + 3w_1,\; c_0 = c_e + c_t + \beta_3 c_s, \tag{9.22}$$

where $\beta_3 > 0$ *is a trace embedding constant depending on* Ω.

Next, we define a convenient right-hand-side function l_{rhs}:

$$l_{\mathrm{rhs}}(P) = (\chi(P), 1)_{\Omega} + w_0 \left(Q_{\Gamma}, P\right)_{\Gamma} + w_1 \left(-\frac{s_0}{3}\boldsymbol{\nu} \otimes \boldsymbol{\nu}, P\right)_{\Gamma}. \tag{9.23}$$

Using (9.20) and (9.23), we can now write $\mathcal{E}[Q]$ in the form

$$\mathcal{E}[Q] = (1/2)b^{i}\left(Q, Q\right) + (1/\eta^2)\left(\psi(Q), 1\right)_{\Omega} + (1/\omega)\left(\phi(Q), 1\right)_{\Gamma} - l_{\mathrm{rhs}}(Q), \tag{9.24}$$

which gives the first variation of $\mathcal{E}$ as:

$$\delta_Q \mathcal{E}[Q; P] = b^{i}\left(Q, P\right) + (1/\eta^2)\left(\psi'(Q), P\right)_{\Omega} + (1/\omega)\left(\phi'(Q), P\right)_{\Gamma} - l_{\mathrm{rhs}}(P). \tag{9.25}$$

9.2. Time-dependent Flow

We consider an evolution equation for Q that is motivated from the Beris–Edwards system [79]. Let $\mathbf{v}$ be the velocity of the liquid crystal fluid domain and assume that $\mathbf{v}$ is divergence free. We introduce the strain and vorticity tensor, respectively,

$$S = S(\nabla \mathbf{v}) := \frac{\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathsf{T}}}{2}, \quad W = W(\nabla \mathbf{v}) := \frac{\nabla \mathbf{v} - (\nabla \mathbf{v})^{\mathsf{T}}}{2}. \tag{9.26}$$

Then, Q evolves by the following parabolic system

$$\begin{aligned} &\partial_t Q + (\mathbf{v} \cdot \nabla) Q + \frac{1}{\tau_0}\widehat{\frac{\delta \mathcal{E}}{\delta Q}} = B\left(\nabla \mathbf{v}, Q\right), \\ &\qquad B\left(\nabla \mathbf{v}, Q\right) := WQ - QW + p_0\left(QS + SQ\right) + \frac{2p_0}{3}S - 2p_0(S : Q)\left(Q + I/3\right), \end{aligned} \tag{9.27}$$

where τ_0 is the relaxation time, $p_0 \in [-1, 1]$ is a material parameter, $\widehat{\cdot}$ is the traceless part, and the boundary conditions come from the weak anchoring conditions. The full strong form is given by

$$\begin{aligned} \partial_t Q + (\mathbf{v} \cdot \nabla) Q - B\left(\nabla \mathbf{v}, Q\right) + \frac{1}{\tau_0}\left(-\mathrm{div}\,\widehat{(\mathcal{A}\nabla Q)} + \frac{1}{\eta^2}\widehat{\psi'(Q)}\right) &= \frac{1}{\tau_0}\widehat{U_{\Omega}}, \quad \text{in } \Omega, \\ \partial_{\boldsymbol{\nu}_{\mathcal{A}}} Q + w_0(Q - Q_{\Gamma}) + w_1(\tilde{Q} - \tilde{Q}^{\perp}) + \frac{1}{\omega}\widehat{\phi'(Q)} &= 0, \quad \text{on } \Gamma, \end{aligned} \tag{9.28}$$

where $\mathcal{A}$ is a 6-tensor such that

$$a_{\mathrm{e}}\left(Q, P\right) + a_{\mathrm{t}}\left(Q, P\right) = \left(\mathcal{A}\nabla Q, \nabla P\right)_{\Omega}.$$

In this case, $Q(x, t)$ satisfies a parabolic PDE (in strong form), and by the standard theory of parabolic PDEs [28, 44], it has a unique solution. The next chapter considers a simplified version of this system for numerical analysis purposes.

Chapter 10. The Modified Allen–Cahn Problem

Before we consider unfitted methods for the Landau–de Gennes model, we first consider the Allen–Cahn equation with some additional nonlinear terms that have properties as the double well terms in (9.28):

$$\begin{aligned} \partial_t y(\cdot,t) + \operatorname{div}(\mathbf{v}y) - \operatorname{div}\,(A\nabla y) + \psi'(y) = f,\ \text{in } \Omega(t),\ \text{for } t>0, \\ \partial_{\boldsymbol{\nu}} y + w_0(y - y_\Gamma) + \phi'(y) = g,\ \text{on } \Gamma(t),\ \text{for } t>0, \end{aligned} \tag{10.1}$$

where f and g are given functions of time and space, $A \in \mathbb{R}^{3\times 3}$ is a symmetric, positive definite matrix, and the material velocity $\mathbf{v}$ is divergence free, i.e. $\nabla\cdot\mathbf{v} = 0$. We note that the analysis for this modified Allen–Cahn equation can be generalized to the analysis for the Landau–de Gennes model.

Additionally, ψ and ϕ are double well functions for the scalar variable $y(\mathbf{x},t)$ that have the same form as in the Landau–de Gennes model and note that ϕ satisfies a scalar version of (9.10) and (9.11) as well. We also assume that $\psi'(0) = \phi'(0) = 0$.

In the following analysis, we consider a convex splitting technique of the double well potentials ψ and ϕ.

$$\begin{aligned} \psi &:= \psi_c - \psi_e \\ \phi &:= \phi_c - \phi_e \end{aligned} \tag{10.2}$$

where ψ_c, ψ_e, ϕ_c, and ϕ_e are all chosen so that each is convex but ψ_e and ϕ_e are quadratic. I.e.

$$\begin{aligned} \psi_e &:= \beta_\psi y^2 \\ \phi_e &:= \beta_\phi y^2 \end{aligned} \tag{10.3}$$

where $\beta_\psi, \beta_\phi > 0$. Furthermore, due to our specific ψ and ϕ, the convex splitting can be performed so that $\psi \geq 0$ and $\phi \geq 0$. We also note that ψ is quartic and has a similar form as (9.7) and that ϕ has quadratic growth like (9.10) and satisfies inequalities (9.11). This will be useful in many of the following proofs in this section.

10.1. Domain Mappings and Extension Operator

Given $u(\boldsymbol{x}, t) : \Omega(t) \to \mathbb{R}$ we assume that there exists an extension operator, say $\mathcal{E}$ such that

$$\mathcal{E}u(\boldsymbol{x}, t) : \mathcal{O}_\delta(\Omega(t)) \to \mathbb{R}, \tag{10.4}$$

and $\mathcal{E}$ has the following properties: For $u \in L^\infty([0,T]; H^{m+1}(\Omega(t))) \cap W^{2,\infty}(\mathcal{Q})$ we have

$$\begin{aligned} \|\mathcal{E}u\|_{H^k(\mathcal{O}_\delta(\Omega(t)))} &\le c_1 \|u\|_{H^k(\Omega(t))}, \quad k = 0, 1, ..., m+1 \\ \|\nabla(\mathcal{E}u)\|_{L^2(\mathcal{O}_\delta(\Omega(t)))} &\le c_2 \|\nabla u\|_{L^2(\Omega(t))}, \\ \|\mathcal{E}u\|_{W^{2,\infty}(\mathcal{O}_\delta(\mathcal{Q}))} &\le c_3 \|u\|_{W^{2,\infty}(\mathcal{Q})}. \end{aligned} \tag{10.5}$$

For $u \in L^\infty([0,T]; H^{m+1}(\Omega(t)))$ with $\partial_t u \in L^\infty([0,T]; H^m(\Omega(t)))$ we have

$$\|\partial_t(\mathcal{E}u)\|_{H^m(\mathcal{O}_\delta(\Omega(t)))} \le c_4 \left(\|u\|_{H^{m+1}(\Omega(t))} + \|\partial_t u\|_{H^m(\Omega(t))} \right). \tag{10.6}$$

See [50] for a proof of the existence of an operator that satisfies these estimates.

Let Ω^n denote the exact domain of (10.1) at a particular time t_n and that Ω_h^n is a high order approximation of Ω^n. To proceed with our analysis, we use assume that Ω^n satisfies Assumption 2 so that we have a geometry approximation Ω_h^n that is of order $q \ge 1$ (i.e. q is the polynomial degree of our level set function) for each n. And we similarly have the same geometry approximation estimate (4.30). Moreover, for each n we assume that there exists a mapping $\boldsymbol{\Phi} : \mathcal{O}_\delta(\Omega^n) \to \mathcal{O}_\delta(\Omega_h^n)$ that satisfies (4.31) and (4.32) where $\boldsymbol{\Phi}$ is a continuous well-defined map that is invertible for sufficiently small h. Note that we have adopted much of the same notation as in Section 4.3.

For any $u : \Omega_h^n \to \mathbb{R}$ in the background finite element space B_h, define $u^\ell := u \circ \mathbf{\Phi}^{-1}$ and note the following estimates:

$$\begin{aligned} \|u^\ell\|^2_{L^2(\mathcal{O}_\delta(\Omega^n))} &\simeq \|u\|^2_{L^2(\mathcal{O}_\delta(\Omega_h^n))} \qquad \|u^\ell\|^2_{L^2(\Omega^n)} \simeq \|u\|^2_{L^2(\Omega_h^n)} \\ \|\nabla u^\ell\|^2_{L^2(\mathcal{O}_\delta(\Omega^n))} &\simeq \|\nabla u\|^2_{L^2(\mathcal{O}_\delta(\Omega_h^n))} \qquad \|\nabla u^\ell\|^2_{L^2(\Omega^n)} \simeq \|\nabla u\|^2_{L^2(\Omega_h^n)} \end{aligned} \tag{10.7}$$

10.2. Semi-discrete Method

We first introduce a time-discretization of the forward problem (10.1). We consider a uniform time step given by $\delta t := T/N$, where T is the final time and N is the number of time steps to be taken. Also, let $t_n := n\delta t$ and denote $y^n := y(t_n)$ with analogous definitions for Ω^n, Γ^n, f^n, g^n, etc. We also use implicit Euler for the time discretization and obtain the following semi-discrete formulation.

$$\begin{aligned} \frac{y^n - y^{n-1}}{\delta t} + (\mathbf{v}\cdot\nabla)y^n - \text{div}\,(A\nabla y^n) + \psi'(y^n) = f^n,\ \text{in } \Omega^n,\ \text{for } n = 1,2,...N, \\ \partial_{\boldsymbol{\nu}} y^n + w_0(y^n - y^n_\Gamma) + \phi'(y^n) = g^n,\ \text{on } \Gamma^n,\ \text{for } n = 1,2,...N, \\ y^0 = h,\ \text{in } \Omega^0. \end{aligned} \tag{10.8}$$

10.2.1. Variational Formulation in Space

The variational formulation for the semi-discrete problem is as follows. Find $y^n \in H^1(\Omega^n)$ such that for all $z \in H^1(\Omega^n)$ we have

$$\begin{aligned} &\int_{\Omega^n} f^n z d\boldsymbol{x} + \int_{\Gamma^n} g^n z dS \\ &\quad = \int_{\Omega^n} \frac{y^n - y^{n-1}}{\delta t} z d\boldsymbol{x} + \frac{1}{2}\int_{\Omega^n} (\mathbf{v}\cdot\nabla y^n)z - (\mathbf{v}\cdot\nabla z)y^n d\boldsymbol{x} + \frac{1}{2}\int_{\Gamma^n} (\boldsymbol{\nu}\cdot\mathbf{v})y^n z dS \\ &\quad\quad + \int_{\Omega^n} (A\nabla y^n)\cdot\nabla z d\boldsymbol{x} + \int_{\Omega^n} \psi'(y) z d\boldsymbol{x} + \int_{\Gamma^n} w_0(y^n - y^n_\Gamma)z + \phi'(y^n) z dS, \end{aligned} \tag{10.9}$$

for each $n = 1, 2, ...N$. Next, we define our linear and bilinear forms as follows:

$$\begin{aligned} a^n(y,z) &= \frac{1}{2}\int_{\Omega^n} (\mathbf{v}\cdot\nabla y)z - (\mathbf{v}\cdot\nabla z)y d\boldsymbol{x} + \int_{\Omega^n} (A\nabla y)\cdot\nabla z d\boldsymbol{x} \\ &\quad + \frac{1}{2}\int_{\Gamma^n} (\boldsymbol{\nu}\cdot\mathbf{v}) yz dS + \int_{\Gamma^n} w_0 yz dS, \\ \chi^n(z) &= \int_{\Omega^n} f^n z d\boldsymbol{x} + \int_{\Gamma^n} g^n z dS + \int_{\Gamma^n} w_0 y_\Gamma^n z dS. \end{aligned} \tag{10.10}$$

Hence, we have the following weak formulation. Find $y^n \in H^1(\Omega^n)$ such that for all $z \in H^1(\Omega^n)$:

$$\int_{\Omega^n} \frac{1}{\delta t} y^n z d\boldsymbol{x} + a^n(y^n, z) + \int_{\Omega^n} \psi'(y^n) z d\boldsymbol{x} + \int_{\Gamma^n} \phi'(y^n) z dS = \chi^n(z) + \int_{\Omega^n} \frac{1}{\delta t} y^{n-1} z d\boldsymbol{x}, \tag{10.11}$$

for each $n = 1, 2, ...N$.

10.2.2. Stability of the Semi-discrete Method

Let us now consider an equivalent problem from the perspective of energy minimization: find $y^n \in H^1(\Omega^n)$ such that

$$\begin{aligned} y^n &= \underset{y\in H^1(\Omega^n)}{\arg\min}\, J^n(y) \\ J^n(y) &:= \frac{1}{2} a^n(y,y) - \chi^n(y) + \int_{\Omega^n} \psi(y) d\boldsymbol{x} + \int_{\Gamma^n} \phi(y) dS + \frac{1}{2\delta t}\|y - y^{n-1}\|^2_{L^2(\Omega^n)}. \end{aligned} \tag{10.12}$$

Lemma 10.1. *The function J^n in* (10.12) *is convex, and hence* (10.11) *and* (10.12) *admit a unique solution, for sufficiently small δt. In particular,*

$$\delta t \le \min\left\{ \frac{1}{4\beta_\psi}, \frac{1}{4}\left(\frac{\beta_\phi^2 C_{\Omega^n}^2}{\alpha} + \frac{\alpha}{4}\right)^{-1}, \frac{1}{4}\left(\frac{C_{\Omega^n}^2(\beta_\phi - C_{\mathbf{v}}/4)^2}{\alpha} + \frac{\alpha}{4}\right)^{-1} \right\},$$

where $\beta_\psi, \beta_\phi > 0$ are terms that come from the convex splitting of ψ and ϕ in (10.3) *and $C_{\mathbf{v}} := \min_{\widehat{\mathfrak{D}}}(2w_0 - |\mathbf{v}|)$.*

Proof.

$$
\begin{aligned}
J^n(y) &= \frac{1}{2}a^n(y,y) - \chi^n(y) + \int_{\Omega^n}\psi(y)d\boldsymbol{x} + \int_{\Gamma^n}\phi(y)dS + \frac{1}{2\delta t}\|y-y^{n-1}\|^2_{L^2(\Omega^n)} \\
&= \frac{1}{2}\int_{\Omega^n}(A\nabla y)\cdot\nabla y d\boldsymbol{x} + \frac{1}{4}\int_{\Gamma^n}(\boldsymbol{\nu}\cdot\mathbf{v})y^2dS + \frac{1}{2}\int_{\Gamma^n}w_0y^2dS - \chi^n(y) \\
&\quad + \int_{\Omega^n}\psi(y)d\boldsymbol{x} + \int_{\Gamma^n}\phi(y)dS + \frac{1}{2\delta t}\|y-y^{n-1}\|^2_{L^2(\Omega^n)}
\end{aligned}
\tag{10.13}
$$

We now use convex splitting of ψ and ϕ and rearrange all the above terms to get the following:

$$
\begin{aligned}
&J^n(y) = J_1^n(y) + J_2^n(y) - \chi^n(y) + \int_{\Omega^n}\psi_c(y)d\boldsymbol{x} + \int_{\Gamma^n}\phi_c(y)dS + \frac{1}{2\delta t}\int_{\Omega^n} -2yy^{n-1} + (y^{n-1})^2 d\boldsymbol{x} \\
&J_1^n(y) := -\int_{\Omega^n}\beta_\psi y^2 d\boldsymbol{x} + \frac{1}{4\delta t}\int_{\Omega^n}y^2 d\boldsymbol{x} \\
&J_2^n(y) := \frac{1}{2}\int_{\Omega^n}(A\nabla y)\cdot\nabla y d\boldsymbol{x} + \frac{1}{4}\int_{\Gamma^n}(\boldsymbol{\nu}\cdot\mathbf{v})y^2dS + \frac{1}{2}\int_{\Gamma^n}w_0y^2dS + \frac{1}{4\delta t}\int_{\Omega^n}y^2d\boldsymbol{x} - \int_{\Gamma^n}\beta_\phi y^2 dS,
\end{aligned}
\tag{10.14}
$$

where all the terms above are trivially convex except for $J_1^n(y)$ and $J_2^n(y)$. We show that for sufficiently small δt, both are convex. Hence, J^n then is also convex. For $J_1^n(y)$, we note that we have the following:

$$
-\int_{\Omega^n}\beta_\psi y^2 d\boldsymbol{x} + \frac{1}{4\delta t}\int_{\Omega^n}y^2 d\boldsymbol{x} = \int_{\Omega^n}\left(\frac{1}{4\delta t} - \beta_\psi\right)y^2 d\boldsymbol{x}, \tag{10.15}
$$

which is convex as long as $\delta t \leq \frac{1}{4\beta_\psi}$. For $J_2^n(y)$, we have

$$
\begin{aligned}
&\frac{1}{2}\int_{\Omega^n}(A\nabla y)\cdot\nabla y d\boldsymbol{x} + \frac{1}{4}\int_{\Gamma^n}(\boldsymbol{\nu}\cdot\mathbf{v})y^2dS + \frac{1}{2}\int_{\Gamma^n}w_0y^2dS + \frac{1}{4\delta t}\int_{\Omega^n}y^2d\boldsymbol{x} - \int_{\Gamma^n}\beta_\phi y^2 dS \\
\geq &\frac{\alpha}{2}\|\nabla y\|^2_{L^2(\Omega^n)} + \frac{1}{4}\int_{\Gamma^n}(2w_0 - |\mathbf{v}|)\,y^2dS + \frac{1}{4\delta t}\int_{\Omega^n}y^2d\boldsymbol{x} - \beta_\phi C_{\Omega^n}\|y\|_{L^2(\Omega^n)}\|y\|_{H^1(\Omega^n)} \\
\geq &\frac{\alpha}{4}\|\nabla y\|^2_{L^2(\Omega^n)} + \frac{C_{\mathbf{v}}}{4}\|y\|^2_{L^2(\Gamma^n)} + \left[\frac{1}{4\delta t} - \frac{\beta_\phi^2 C_{\Omega^n}^2}{\alpha} - \frac{\alpha}{4}\right]\|y\|^2_{L^2(\Omega^n)},
\end{aligned}
\tag{10.16}
$$

where we have used a trace estimate and a weighted Young's inequality. We also notice that if $C_{\mathbf{v}} := \min_{\widehat{\mathfrak{D}}} (2w_0 - |\mathbf{v}|) \geq 0$ then (10.16) is convex as long as

$$\delta t \leq \frac{1}{4}\left(\frac{\beta_\phi^2 C_{\Omega^n}^2}{\alpha} + \frac{\alpha}{4}\right)^{-1}.$$

Otherwise, analogous arguments show that we need the restriction

$$\delta t \leq \frac{1}{4}\left(\frac{C_{\Omega^n}^2(\beta_\phi - C_{\mathbf{v}}/4)^2}{\alpha} + \frac{\alpha}{4}\right)^{-1}.$$

□

Lemma 10.2. *We have the following estimate for controlling the double well potentials. Additionally, if δt is chosen sufficiently small we have coercivity in* (10.11)*. Hence, $\forall y \in H^1(\Omega^n)$ we have,*

$$a^n(y,y) + \int_{\Omega^n} \psi'(y) y d\boldsymbol{x} + \int_{\Gamma^n} \phi'(y) y dS \geq \frac{\alpha}{2}\|\nabla y\|_{L^2(\Omega^n)}^2 - \zeta'\|y\|_{L^2(\Omega^n)}^2 \tag{10.17}$$

where $\zeta' = \left[\frac{C_{\Omega^n}^2\zeta^2}{2\alpha} + \frac{\alpha}{2} + 2\beta_\psi\right]$ and $\zeta = 2\beta_\phi + \frac{1}{2}\|\boldsymbol{\nu}\cdot\mathbf{v}\|_{L^\infty(\Gamma^n)}$ where β_ψ and β_ϕ come from convex splitting in (10.3)*.*

Proof.

$$\begin{aligned}
&a^n(y,y) + \int_{\Omega^n} \psi'(y) y d\boldsymbol{x} + \int_{\Gamma^n} \phi'(y) y dS \\
&\quad = \frac{1}{2}\int_{\Gamma^n} (\boldsymbol{\nu}\cdot\mathbf{v}) y^2 dS + \int_{\Omega^n} (A\nabla y)\cdot\nabla y d\boldsymbol{x} + \int_{\Omega^n} \psi'(y) y d\boldsymbol{x} + \int_{\Gamma^n} w_0 y^2 + \phi'(y) y dS \\
&\quad \geq \alpha\|\nabla y\|_{L^2(\Omega^n)}^2 + \frac{1}{2}\int_{\Gamma^n} (\boldsymbol{\nu}\cdot\mathbf{v}) y^2 dS + \int_{\Omega^n} \psi'(y) y d\boldsymbol{x} + \int_{\Gamma^n} w_0 y^2 + \phi'(y) y dS \\
&\quad \geq \alpha\|\nabla y\|_{L^2(\Omega^n)}^2 - \frac{1}{2}\|\boldsymbol{\nu}\cdot\mathbf{v}\|_{L^\infty(\Gamma^n)}\|y\|_{L^2(\Gamma^n)}^2 + \int_{\Omega^n} \psi'(y) y d\boldsymbol{x} + \int_{\Gamma^n} \phi'(y) y dS
\end{aligned} \tag{10.18}$$

where we have used the fact that the matrix A is symmetric positive definite and hence we find that it is strongly elliptic ($v^T A v \geq \alpha\|v\|^2$ and $\alpha > 0$). We will also recall one of the convexity properties to find that $0 \le [\psi_c'(y) - \psi_c'(0)](y-0)$ with analogous property for ϕ_c.

So now we have the following:

$$
\begin{aligned}
&a^n(y,y) + \int_{\Omega^n} \psi'(y) y d\boldsymbol{x} + \int_{\Gamma^n} \phi'(y) y dS \\
&\quad \ge \alpha \|\nabla y\|^2_{L^2(\Omega^n)} - \frac{1}{2}\|\boldsymbol{\nu}\cdot\mathbf{v}\|_{L^\infty(\Gamma^n)}\|y\|^2_{L^2(\Gamma^n)} + \int_{\Omega^n} \psi_c'(y)y - \psi_e'(y) y d\boldsymbol{x} + \int_{\Gamma^n} \phi_c'(y)y - \phi_e'(y)ydS \\
&\quad \ge \alpha \|\nabla y\|^2_{L^2(\Omega^n)} - \left[2\beta_\phi + \frac{1}{2}\|\boldsymbol{\nu}\cdot\mathbf{v}\|_{L^\infty(\Gamma^n)}\right]\|y\|^2_{L^2(\Gamma^n)} + \int_{\Omega^n}[\psi_c'(y) - \psi_c'(0)](y-0) - 2\beta_\psi y^2 d\boldsymbol{x} \\
&\qquad\qquad + \int_{\Gamma^n}[\phi_c'(y) - \phi_c'(0)](y-0) dS \\
&\quad \ge \alpha \|\nabla y\|^2_{L^2(\Omega^n)} - \left[2\beta_\phi + \frac{1}{2}\|\boldsymbol{\nu}\cdot\mathbf{v}\|_{L^\infty(\Gamma^n)}\right]\|y\|^2_{L^2(\Gamma^n)} - \int_{\Omega^n} 2\beta_\psi y^2 d\boldsymbol{x} \\
&\quad \ge \alpha \|\nabla y\|^2_{L^2(\Omega^n)} - C_{\Omega^n}\zeta\|y\|_{L^2(\Omega^n)}\|y\|_{H^1(\Omega^n)} - 2\beta_\psi\|y\|^2_{L^2(\Omega^n)} \\
&\quad \ge \alpha \|\nabla y\|^2_{L^2(\Omega^n)} - \frac{C^2_{\Omega^n}\zeta^2}{2\alpha}\|y\|^2_{L^2(\Omega^n)} - \frac{\alpha}{2}\|y\|^2_{H^1(\Omega^n)} - 2\beta_\psi\|y\|^2_{L^2(\Omega^n)} \\
&\quad = \frac{\alpha}{2}\|\nabla y\|^2_{L^2(\Omega^n)} - \left[\frac{C^2_{\Omega^n}\zeta^2}{2\alpha} + \frac{\alpha}{2} + 2\beta_\psi\right]\|y\|^2_{L^2(\Omega^n)}
\end{aligned}
\tag{10.19}
$$

where $\zeta = 2\beta_\phi + \frac{1}{2}\|\boldsymbol{\nu}\cdot\mathbf{v}\|_{L^\infty(\Gamma^n)}$ and we have what we wanted to show. □

Lemma 10.3. *Let y^n solve* (10.11) *for $n = 1, 2, ...N$. Then, we have the following stability estimate:*

$$
\|y^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{2}\delta t \sum_{n=1}^{k} \|\nabla y^n\|^2_{L^2(\Omega^n)} \le 2\left(D + C_1\|y^0\|^2_{L^2(\Omega^0)}\right)\exp((C_2 + \zeta'')2t_k), \tag{10.20}
$$

where $D = \delta t \sum_{n=1}^{N}\left[\|f^n\|^2_{L^2(\Omega^n)} + \|g^n + w_0 y^n_\Gamma\|^2_{L^2(\Gamma^n)}\right]$.

Proof. Recall (10.11)

$$
\int_{\Omega^n} \frac{1}{\delta t} y^n z d\boldsymbol{x} + a^n(y^n, z) + \int_{\Omega^n}\psi'(y^n) z d\boldsymbol{x} + \int_{\Gamma^n}\phi'(y^n) z dS = \chi^n(z) + \int_{\Omega^n}\frac{1}{\delta t} y^{n-1} z d\boldsymbol{x}, \tag{10.21}
$$

and choose $z = 2\delta t y^n$ so that we get

$$
\begin{aligned}
&2\|y^n\|^2_{L^2(\Omega^n)} + 2\delta t a^n(y^n, y^n) + 2\delta t \int_{\Omega^n} \psi'(y^n) y^n d\boldsymbol{x} + 2\delta t \int_{\Gamma^n} \phi'(y^n) y^n dS \\
&\qquad = 2\delta t \chi^n(y^n) + \int_{\Omega^n} 2y^{n-1} y^n d\boldsymbol{x}.
\end{aligned}
\tag{10.22}
$$

And now, rearranging terms and applying Lemma 10.2, we obtain the following:

$$
(1 - 2\delta t\zeta')\|y^n\|^2_{L^2(\Omega^n)} + \alpha\delta t\|\nabla y^n\|^2_{L^2(\Omega^n)} \leq 2\delta t\chi^n(y^n) + \|y^{n-1}\|^2_{L^2(\Omega^n)}, \tag{10.23}
$$

where we estimate $\chi^n(y^n)$ as follows:

$$
\begin{aligned}
\chi^n(y^n) &= \int_{\Omega^n} f^n y^n d\boldsymbol{x} + \int_{\Gamma^n} (g^n + w_0 y^n_\Gamma) y^n dS \\
&\leq \|f^n\|_{L^2(\Omega^n)}\|y^n\|_{L^2(\Omega^n)} + \|g^n + w_0 y^n_\Gamma\|_{L^2(\Gamma^n)}\|y^n\|_{L^2(\Gamma^n)} \\
&\leq \frac{1}{2}\|f^n\|^2_{L^2(\Omega^n)} + \frac{1}{2}\|y^n\|^2_{L^2(\Omega^n)} + \frac{1}{2}\|g^n + w_0 y^n_\Gamma\|^2_{L^2(\Gamma^n)} + \frac{1}{2}\|y^n\|^2_{L^2(\Gamma^n)} \\
&\leq \frac{1}{2}\|f^n\|^2_{L^2(\Omega^n)} + \frac{1}{2}\|y^n\|^2_{L^2(\Omega^n)} + \frac{1}{2}\|g^n + w_0 y^n_\Gamma\|^2_{L^2(\Gamma^n)} + \frac{C_{\Omega^n}}{2}\|y^n\|_{L^2(\Omega^n)}\|y^n\|_{H^1(\Omega^n)} \\
&\leq \frac{1}{2}\|f^n\|^2_{L^2(\Omega^n)} + \frac{1}{2}\|g^n + w_0 y^n_\Gamma\|^2_{L^2(\Gamma^n)} + \left[\frac{C^2_{\Omega^n}}{4\alpha} + \frac{\alpha}{4} + \frac{1}{2}\right]\|y^n\|^2_{L^2(\Omega^n)} + \frac{\alpha}{4}\|\nabla y^n\|^2_{L^2(\Omega^n)}.
\end{aligned}
\tag{10.24}
$$

So then, by combining (10.23) and the above estimate, we get

$$
\begin{aligned}
(1 - \delta t\zeta'')\|y^n\|^2_{L^2(\Omega^n)} + \frac{\alpha}{2}\delta t\|\nabla y^n\|^2_{L^2(\Omega^n)} &\leq \delta t\|f^n\|^2_{L^2(\Omega^n)} \\
&\quad + \delta t\|g^n + w_0 y^n_\Gamma\|^2_{L^2(\Gamma^n)} + \|y^{n-1}\|^2_{L^2(\Omega^n)},
\end{aligned}
\tag{10.25}
$$

where $\zeta'' = \left[2\zeta' + \frac{C^2_{\Omega^n}}{2\alpha} + \frac{\alpha}{2} + 1\right]$. Now using Lemmas 3.4 and 3.5 from [50], we get the following estimates for $\|y^{n-1}\|^2_{L^2(\Omega^n)}$:

$$
\begin{aligned}
&\|y^0\|^2_{L^2(\Omega^1)} \leq \|y^0\|^2_{L^2(\mathcal{O}_\delta(\Omega^0))} \leq C_1\|y^0\|^2_{L^2(\Omega^0)}, \\
&\|y^{n-1}\|^2_{L^2(\Omega^n)} \leq \|y^{n-1}\|^2_{L^2(\mathcal{O}_\delta(\Omega^{n-1}))} \leq (1 + C_2\delta t)\|y^{n-1}\|^2_{L^2(\Omega^{n-1})} + \frac{\alpha}{4}\delta t\|\nabla y^{n-1}\|^2_{L^2(\Omega^{n-1})}.
\end{aligned}
\tag{10.26}
$$

Now, by summing up (10.25) over $n = 1, ..., k$, we get the following:

$$\begin{aligned}(1-\delta t\zeta'')\sum_{n=1}^{k}\|y^n\|^2_{L^2(\Omega^n)} + \frac{\alpha}{2}\delta t\sum_{n=1}^{k}\|\nabla y^n\|^2_{L^2(\Omega^n)}\\ \leq \delta t\sum_{n=1}^{k}\left[\|f^n\|^2_{L^2(\Omega^n)} + \|g^n + w_0 y^n_\Gamma\|^2_{L^2(\Gamma^n)}\right] + \sum_{n=1}^{k}\|y^{n-1}\|^2_{L^2(\Omega^n)}.\end{aligned} \tag{10.27}$$

We now apply (10.26) to each term in $\sum_{n=1}^{k}\|y^{n-1}\|^2_{L^2(\Omega^n)}$ and reorder to get

$$\begin{aligned}(1-\delta t\zeta'')\|y^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{4}\delta t\sum_{n=1}^{k}\|\nabla y^n\|^2_{L^2(\Omega^n)}\\ \leq D + C_1\|y^0\|^2_{L^2(\Omega^0)} + \sum_{n=0}^{k-1}\delta t(C_2+\zeta'')\|y^n\|^2_{L^2(\Omega^n)},\end{aligned} \tag{10.28}$$

where $D = \delta t\sum_{n=1}^{N}\left[\|f^n\|^2_{L^2(\Omega^n)} + \|g^n + w_0 y^n_\Gamma\|^2_{L^2(\Gamma^n)}\right]$ is the initial data. By choosing δt sufficiently small so that $(1-\delta t\zeta'') \geq \frac{1}{2}$ we get

$$\frac{1}{2}\|y^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{4}\delta t\sum_{n=1}^{k}\|\nabla y^n\|^2_{L^2(\Omega^n)} \leq D + C_1\|y^0\|^2_{L^2(\Omega^0)} + \sum_{n=0}^{k-1}\delta t(C_2+\zeta'')\|y^n\|^2_{L^2(\Omega^n)}. \tag{10.29}$$

And by the discrete Gronwall inequality stated in Lemma 1 of the appendix, we get the assertion:

$$\|y^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{2}\delta t\sum_{n=1}^{k}\|\nabla y^n\|^2_{L^2(\Omega^n)} \leq 2\left(D + C_1\|y^0\|^2_{L^2(\Omega^0)}\right)\exp((C_2+\zeta'')2t_k). \tag{10.30}$$

□

10.3. Discretization in Time and Space

The Unfitted Finite Element Scheme

We define the background finite element space B_h and the restricted finite element space V_h in the same way as (3.7) and (3.16) but state it again.

$$\begin{aligned}B_h =& \{\boldsymbol{v}_h \in C^0(\widehat{\mathfrak{D}}) : \boldsymbol{v}_h|_T \in \mathcal{P}_k(T),\ \forall T \in \widehat{\mathcal{T}}_h\}, \quad \text{for some } k \geq 1.\\ V_h \equiv& V_h(\Omega_h) = \{\boldsymbol{v}_h \in C^0(\mathfrak{D}_{h,\delta}) : \boldsymbol{v}_h = \hat{\boldsymbol{v}}_h|_{\mathfrak{D}_{h,\delta}},\ \text{for some } \hat{\boldsymbol{v}}_h \in B_h\},\end{aligned} \tag{10.31}$$

i.e. $V_h = B_h|_{\mathfrak{D}_{h,\delta}}$. We recall from Section 3.3 that the unfitted approach requires a special facet stabilization term which we previously defined in (3.17) and (3.18)

We use an implicit Euler method to approximate the time derivative and we derive the variational formulation of the Allen–Cahn PDE in (10.1) to obtain:

$$\begin{aligned}
&\int_{\Omega_h^n} f_h^n z_h d\boldsymbol{x} + \int_{\Gamma_h^n} g_h^n z_h dS \\
&\quad = \int_{\Omega_h^n} \frac{y_h^n - y_h^{n-1}}{\delta t} z_h d\boldsymbol{x} + \frac{1}{2}\int_{\Omega_h^n} (\mathbf{v}\cdot\nabla y_h^n) z_h - (\mathbf{v}\cdot\nabla z_h) y_h^n d\boldsymbol{x} + \frac{1}{2}\int_{\Gamma_h^n} (\boldsymbol{\nu}\cdot\mathbf{v}) y_h^n z_h dS \\
&\qquad + \int_{\Omega_h^n} (A\nabla y_h^n)\cdot\nabla z_h d\boldsymbol{x} + \int_{\Omega_h^n} \psi'(y_h^n) z_h d\boldsymbol{x} + \int_{\Gamma_h^n} w_0 (y_h^n - y_{\Gamma,h}^n) z_h + \phi'(y_h^n) z_h dS,
\end{aligned} \tag{10.32}$$

where $y_{\Gamma,h}^n$, f_h^n, and g_h^n are the interpolants of y_Γ^n, f^n, and g^n respectively that have been suitably extended such that the following estimates hold:

$$\begin{aligned}
\|f_h^n - f^n\|_{H^1(\mathcal{O}(\Omega^n))} &\approx h^q \\
\|g_h^n - g^n\|_{H^1(\Gamma_h^n)} &\approx h^q \\
\|y_{\Gamma,h}^n - y_\Gamma^n\|_{H^1(\Gamma_h^n)} &\approx h^q,
\end{aligned} \tag{10.33}$$

on some extended region $\mathcal{O}(\Omega^n)$ that contains Ω_h^n. Also, $\mathbf{v}$ is a suitable extension on $\mathcal{O}(\Omega^n)$ and for simplicity we assume that $\mathbf{v}$ is defined on the entire design domain.

Next, we define the following linear and bilinear forms

$$\begin{aligned}
a_h^n(y,z) &= \frac{1}{2}\int_{\Omega_h^n} (\mathbf{v}\cdot\nabla y) z - (\mathbf{v}\cdot\nabla z) y d\boldsymbol{x} + \int_{\Omega_h^n} (A\nabla y)\cdot\nabla z d\boldsymbol{x} \\
&\qquad + \frac{1}{2}\int_{\Gamma_h^n} (\boldsymbol{\nu}\cdot\mathbf{v}) y z dS + \int_{\Gamma_h^n} w_0 y z dS \\
A_h^n(y,z) &= a_h^n(y,z) + \gamma_s s_h(\mathcal{F}_{\Sigma_\delta^\pm}^n; y, z) \\
\chi_h^n(z) &= \int_{\Omega_h^n} f_h^n z d\boldsymbol{x} + \int_{\Gamma_h^n} g_h^n z dS + \int_{\Gamma_h^n} w_0 y_{\Gamma,h}^n z dS
\end{aligned} \tag{10.34}$$

where $\gamma_{\mathrm{s}} > 0$. And so the unfitted finite element scheme is as follows: Find $y_h^n \in V_h(\Omega_h^n)$ such that for all $z_h \in V_h(\Omega_h^n)$ we have

$$\int_{\Omega_h^n} \frac{y_h^n}{\delta t} z_h d\boldsymbol{x} + A_h^n\left(y_h^n, z_h\right) + \int_{\Omega_h^n} \psi'(y_h^n) z_h d\boldsymbol{x} + \int_{\Gamma_h^n} \phi'(y_h^n) z_h dS = \chi_h^n\left(z\right) + \int_{\Omega_h^n} \frac{y_h^{n-1}}{\delta t} z_h d\boldsymbol{x} \tag{10.35}$$

for each $n = 1, 2, ..., N$.

10.3.1. Coercivity of the Fully Discrete Method

Lemma 10.4. *Assume that $\psi'(0) = \phi'(0) = 0$ and that the convex splitting in* (10.2) *was done so that $\phi_c \geq 0$ and $\psi_c \geq 0$. Then we have the following estimate for controlling the double well potentials. Additionally, if δt is chosen sufficiently small we have coercivity in* (10.35)*. Hence, $\forall y_h^n \in H^1(\Omega_h^n)$ we have,*

$$a_h^n\left(y_h^n, y_h^n\right) + \int_{\Omega_h^n} \psi'(y_h^n) y_h^n d\boldsymbol{x} + \int_{\Gamma_h^n} \phi'(y_h^n) y_h^n dS \geq \frac{\alpha}{2} \|\nabla y_h^n\|^2_{L^2(\Omega_h^n)} - \zeta_h' \|y_h^n\|^2_{L^2(\Omega_h^n)} \tag{10.36}$$

where $\zeta_h' = \left[\frac{C^2_{\Omega_h^n}\zeta_h^2}{2\alpha} + \frac{\alpha}{2} + 2\beta_\psi\right]$ and $\zeta_h = 2\beta_\phi + \frac{1}{2}\|\boldsymbol{\nu}\cdot\mathbf{v}\|_{L^\infty(\Gamma_h^n)}$ where β_ψ and β_ϕ come from convex splitting in (10.3)*.*

Proof. This is the same proof from Lemma 10.2. □

10.4. Error Analysis for the Fully Discrete Method

We give a brief overview of the error analysis for the approximation of the weak form. We make the same assumption as earlier (Assumption 1) and recall the previous inverse estimates from Proposition 4.2.

10.4.1. Stability of the Fully Discrete Method

Theorem 10.5. *Let y^n solve* (10.35) *for $n = 1, 2, ...N$. Then, we have the following stability estimate:*

$$\begin{aligned} &\|y^k\|^2_{L^2(\Omega_h^k)} + \frac{\alpha}{4}\delta t \sum_{n=1}^{k} \|\nabla y_h^n\|^2_{L^2(\Omega_h^n)} \\ &\quad \leq \exp((C_2 + \zeta_h'')t_k) \left(D + C_1 \|y^0\|^2_{L^2(\Omega_h^0)} + C_1 K h^2 s_h(\mathcal{F}^0_{\Sigma_\delta^\pm}; y_h^0, y_h^0) \right) \end{aligned} \tag{10.37}$$

where $D = C_I \delta t \sum_{n=1}^{N} \left[\|f^n\|^2_{L^2(\Omega_h^n)} + \|g^n + w_0 y_\Gamma^n\|^2_{L^2(\Gamma_h^n)} \right]$ and C_1, C_2 are constants that depend on the estimates of the extension operator and C_I is a constant that depends on the interpolation of the initial data.

Proof. Recall (10.35):

$$\int_{\Omega_h^n} \frac{y_h^n}{\delta t} z_h d\boldsymbol{x} + A_h^n(y_h^n, z_h) + \int_{\Omega_h^n} \psi'(y_h^n) z_h d\boldsymbol{x} + \int_{\Gamma_h^n} \phi'(y_h^n) z_h dS = \chi_h^n(z) + \int_{\Omega_h^n} \frac{y_h^{n-1}}{\delta t} z_h d\boldsymbol{x}, \tag{10.38}$$

and choose $z_h = 2\delta t y_h^n$ so that we get

$$\begin{aligned} &2\|y_h^n\|^2_{L^2(\Omega_h^n)} + 2\delta t A_h^n(y_h^n, y_h^n) + 2\delta t \int_{\Omega_h^n} \psi'(y_h^n) y_h^n d\boldsymbol{x} + 2\delta t \int_{\Gamma_h^n} \phi'(y_h^n) y_h^n dS \\ &\quad = 2\delta t \chi_h^n(y_h^n) + \int_{\Omega_h^n} 2 y_h^{n-1} y_h^n d\boldsymbol{x}. \end{aligned} \tag{10.39}$$

Next, by rearranging terms and using Lemma 10.4, we get the following:

$$(1 - 2\delta t \zeta_h')\|y_h^n\|^2_{L^2(\Omega_h^n)} + \alpha \delta t \|\nabla y_h^n\|^2_{L^2(\Omega_h^n)} + 2\delta t \gamma_{\mathrm{s}} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; y_h^n, y_h^n) \leq 2\delta t \chi_h^n(y_h^n) + \|y_h^{n-1}\|^2_{L^2(\Omega_h^n)}. \tag{10.40}$$

Now notice that we can estimate $\chi_h^n(y_h^n)$ as follows:

$$\begin{aligned}
\chi_h^n(y_h^n) &= \int_{\Omega_h^n} f_h^n y_h^n d\boldsymbol{x} + \int_{\Gamma_h^n} (g_h^n + w_0 y_{\Gamma,h}^n) y_h^n dS \\
&\leq \|f_h^n\|_{L^2(\Omega_h^n)} \|y_h^n\|_{L^2(\Omega_h^n)} + \|g_h^n + w_0 y_{\Gamma,h}^n\|_{L^2(\Gamma_h^n)} \|y_h^n\|_{L^2(\Gamma_h^n)} \\
&\leq \frac{1}{2}\|f_h^n\|^2_{L^2(\Omega_h^n)} + \frac{1}{2}\|y_h^n\|^2_{L^2(\Omega_h^n)} + \frac{1}{2}\|g_h^n + w_0 y_{\Gamma,h}^n\|^2_{L^2(\Gamma_h^n)} + \frac{1}{2}\|y_h^n\|^2_{L^2(\Gamma_h^n)} \\
&\leq \frac{C_I}{2}\|f^n\|^2_{L^2(\Omega_h^n)} + \frac{1}{2}\|y_h^n\|^2_{L^2(\Omega_h^n)} + \frac{C_I}{2}\|g^n + w_0 y_\Gamma^n\|^2_{L^2(\Gamma_h^n)} + \frac{C_{\Omega_h^n}}{2}\|y_h^n\|_{L^2(\Omega_h^n)} \|y_h^n\|_{H^1(\Omega_h^n)} \\
&\leq \frac{C_I}{2}\|f^n\|^2_{L^2(\Omega_h^n)} + \frac{C_I}{2}\|g^n + w_0 y_\Gamma^n\|^2_{L^2(\Gamma_h^n)} + \left[\frac{C^2_{\Omega_h^n}}{4\alpha} + \frac{\alpha}{4} + \frac{1}{2}\right]\|y_h^n\|^2_{L^2(\Omega_h^n)} + \frac{\alpha}{4}\|\nabla y_h^n\|^2_{L^2(\Omega_h^n)},
\end{aligned} \tag{10.41}$$

where C_I is the constant corresponding to the interpolation estimate of the initial data. So, then by combining (10.23) and the above estimate, we get

$$\begin{aligned}
(1 - \delta t \zeta_h'') \|y_h^n\|^2_{L^2(\Omega_h^n)} + \frac{\alpha}{2}\delta t \|\nabla y_h^n\|^2_{L^2(\Omega_h^n)} + 2\delta t \gamma_s s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; y_h^n, y_h^n) \\
\leq C_I \delta t \|f^n\|^2_{L^2(\Omega_h^n)} + C_I \delta t \|g^n + w_0 y_\Gamma^n\|^2_{L^2(\Gamma_h^n)} + \|y_h^{n-1}\|^2_{L^2(\Omega_h^n)}
\end{aligned} \tag{10.42}$$

where $\zeta_h'' = \left[2\zeta_h' + \frac{C^2_{\Omega_h^n}}{2\alpha} + \frac{\alpha}{2} + 1\right]$. And now using Lemmas 5.5 and 5.7 from [50], we get the following estimates for $\|y_h^{n-1}\|^2_{L^2(\Omega_h^n)}$ that hold for all $1 \leq n \leq N$ for constants C_1, C_2, C_3 that do not depend on n:

$$\begin{aligned}
\|y_h^0\|^2_{L^2(\Omega_h^1)} &\leq \|y_h^0\|^2_{L^2(\mathcal{O}_\delta(\Omega_h^0)} \leq C_1 \|y_h^0\|^2_{L^2(\Omega_h^0)} + C_1 K h^2 s_h(\mathcal{F}^0_{\Sigma_\delta^\pm}; y_h^0, y_h^0) \\
\|y_h^{n-1}\|^2_{L^2(\Omega_h^n)} &\leq \|y_h^{n-1}\|^2_{L^2(\mathcal{O}_\delta(\Omega_h^{n-1})} \\
&\leq (1 + C_2 \delta t)\|y_h^{n-1}\|^2_{L^2(\Omega_h^{n-1})} + \frac{\alpha}{4}\delta t \|\nabla y_h^{n-1}\|^2_{L^2(\Omega_h^{n-1})} + C_3 \delta t K s_h(\mathcal{F}^{n-1}_{\Sigma_\delta^\pm}; y_h^{n-1}, y_h^{n-1}).
\end{aligned} \tag{10.43}$$

Now, choosing $\gamma_s \geq C_3 K$ and by summing up (10.42) over $n = 1, ..., k$, we get the following:

$$\begin{aligned}(1-\delta t\zeta_h'')\sum_{n=1}^{k}\|y_h^n\|^2_{L^2(\Omega_h^n)}+\frac{\alpha}{2}\delta t\sum_{n=1}^{k}\|\nabla y_h^n\|^2_{L^2(\Omega_h^n)}+2\delta t\gamma_{\mathrm{s}}\sum_{n=1}^{k}s_h(\mathcal{F}^n_{\Sigma_\delta^\pm};y_h^n,y_h^n)\\ \le C_I\delta t\sum_{n=1}^{k}\left[\|f^n\|^2_{L^2(\Omega_h^n)}+\|g^n+w_0y_\Gamma^n\|^2_{L^2(\Gamma_h^n)}\right]+\sum_{n=1}^{k}\|y_h^{n-1}\|^2_{L^2(\Omega_h^n)}.\end{aligned} \tag{10.44}$$

We now apply (10.43) to each term in $\sum_{n=1}^{k}\|y_h^{n-1}\|^2_{L^2(\Omega_h^n)}$ and reorder to get

$$\begin{aligned}(1-\delta t\zeta_h'')\,\|y^k\|^2_{L^2(\Omega_h^k)}+\frac{\alpha}{4}\delta t\sum_{n=1}^{k}\|\nabla y_h^n\|^2_{L^2(\Omega_h^n)}+\delta t\gamma_{\mathrm{s}}\sum_{n=1}^{k}s_h(\mathcal{F}^n_{\Sigma_\delta^\pm};y_h^n,y_h^n)\\ \le\delta t\sum_{n=2}^{k}\left[(C_2+\zeta_h'')\|y_h^{n-1}\|^2_{L^2(\Omega_h^{n-1})}\right]+D+C_1\|y^0\|^2_{L^2(\Omega_h^0)}+C_1Kh^2s_h(\mathcal{F}^0_{\Sigma_\delta^\pm};y_h^0,y_h^0),\end{aligned} \tag{10.45}$$

where $D=C_I\delta t\sum_{n=1}^{N}\left[\|f^n\|^2_{L^2(\Omega_h^n)}+\|g^n+w_0y_\Gamma^n\|^2_{L^2(\Gamma_h^n)}\right]$ is the initial data. And by choosing δt sufficiently small so that $(1-\delta t\zeta_h'')\ge\frac{1}{2}$ we have

$$\begin{aligned}\frac{1}{2}\|y^k\|^2_{L^2(\Omega_h^k)}+\frac{\alpha}{4}\delta t\sum_{n=1}^{k}\|\nabla y_h^n\|^2_{L^2(\Omega_h^n)}+\delta t\gamma_{\mathrm{s}}\sum_{n=1}^{k}s_h(\mathcal{F}^n_{\Sigma_\delta^\pm};y_h^n,y_h^n)\\ \le\delta t\sum_{n=2}^{k}\left[(C_2+\zeta_h'')\|y_h^{n-1}\|^2_{L^2(\Omega_h^{n-1})}\right]+D+C_1\|y^0\|^2_{L^2(\Omega_h^0)}+C_1Kh^2s_h(\mathcal{F}^0_{\Sigma_\delta^\pm};y_h^0,y_h^0).\end{aligned} \tag{10.46}$$

And by the discrete Gronwall inequality stated in Lemma 1 of the appendix, we get the assertion:

$$\begin{aligned}\|y^k\|^2_{L^2(\Omega_h^k)}+\delta t\sum_{n=1}^{k}\left[\frac{\alpha}{2}\|\nabla y_h^n\|^2_{L^2(\Omega_h^n)}+\gamma_{\mathrm{s}}\sum_{n=1}^{k}s_h(\mathcal{F}^n_{\Sigma_\delta^\pm};y_h^n,y_h^n)\right]\\ \le 2\left(D+C_1\|y^0\|^2_{L^2(\Omega_h^0)}+C_1Kh^2s_h(\mathcal{F}^0_{\Sigma_\delta^\pm};y_h^0,y_h^0)\right)\exp((C_2+\zeta_h'')2t_k).\end{aligned} \tag{10.47}$$

□

10.4.2. Consistency Estimate

Taking (10.11) before the approximation of the time derivative we get:

$$\int_{\Omega^n}[\partial_t y^n]z\,d\boldsymbol{x}+a^n\left(y^n,z\right)+\int_{\Omega^n}\psi'(y^n)z\,d\boldsymbol{x}+\int_{\Gamma^n}\phi'(y^n)z\,dS=\chi^n\left(z\right)\quad\forall z\in H^1(\Omega^n), \tag{10.48}$$

and we choose $z = z_h^\ell := z_h \circ \mathbf{\Phi}^{-1}$ for arbitrary $z_h \in V_h(\Omega_h^n)$. Now also recall the fully discrete formulation:

$$\int_{\Omega_h^n} \frac{y_h^n - y_h^{n-1}}{\delta t} z_h d\boldsymbol{x} + A_h^n\left(y_h^n, z_h\right) + \int_{\Omega_h^n} \psi'(y_h^n) z_h d\boldsymbol{x} + \int_{\Gamma_h^n} \phi'(y_h^n) z_h dS = \chi_h^n\left(z_h\right). \tag{10.49}$$

Now, taking the difference between (10.48) and the fully discretized problem (10.49), we get the following:

$$\begin{aligned}
&\int_{\Omega_h^n} \frac{\mathbb{E}^n - \mathbb{E}^{n-1}}{\delta t} z_h d\boldsymbol{x} + a_h^n\left(\mathbb{E}^n, z_h\right) + \gamma_{\mathrm{s}} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; \mathbb{E}^n, z_h) \\
&\qquad = \mathcal{E}_0(z_h) + \int_{\Omega_h^n} \psi'(y_h^n) z_h d\boldsymbol{x} - \int_{\Omega^n} \psi'(y^n) z_h^\ell d\boldsymbol{x} + \int_{\Gamma_h^n} \phi'(y_h^n) z_h dS - \int_{\Gamma^n} \phi'(y^n) z_h^\ell dS,
\end{aligned} \tag{10.50}$$

where we have the following definitions

$$\begin{aligned}
\mathbb{E}^n &:= y^n - y_h^n \quad \forall n, \\
\mathcal{E}_0(z_h) &:= \mathcal{E}_1(z_h) + \mathcal{E}_2(z_h) + \mathcal{E}_3(z_h) + \mathcal{E}_4(z_h), \\
\mathcal{E}_1(z_h) &:= \int_{\Omega_h^n} \frac{y^n - y^{n-1}}{\delta t} z_h d\boldsymbol{x} - \int_{\Omega^n} [\partial_t y^n] z_h^\ell d\boldsymbol{x}, \\
\mathcal{E}_2(z_h) &:= a_h^n\left(y^n, z_h\right) - a^n\left(y^n, z_h^\ell\right), \\
\mathcal{E}_3(z_h) &:= \gamma_{\mathrm{s}} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; y^n, z_h), \\
\mathcal{E}_4(z_h) &:= \chi^n\left(z_h^\ell\right) - \chi_h^n\left(z_h\right), \\
\mathcal{E}_\psi(z_h) &:= \int_{\Omega_h^n} \psi'(y_h^n) z_h d\boldsymbol{x} - \int_{\Omega^n} \psi'(y^n) z_h^\ell d\boldsymbol{x}, \\
\mathcal{E}_\phi(z_h) &:= \int_{\Gamma_h^n} \phi'(y_h^n) z_h dS - \int_{\Gamma^n} \phi'(y^n) z_h^\ell dS.
\end{aligned} \tag{10.51}$$

We further split (10.50) using the lagrange interpolant of y^n denoted by $y_I^n \in V_h(\Omega_h^n)$ given that y^n is sufficiently smooth. Next, define

$$\mathbb{E}^n := \underbrace{y^n - y_I^n}_{e^n} + \underbrace{y_I^n - y_h^n}_{e_h^n \in V_h(\Omega_h^n)} \quad \forall n. \tag{10.52}$$

Then, we get the following

$$\int_{\Omega_h^n} \frac{e_h^n - e_h^{n-1}}{\delta t} z_h d\boldsymbol{x} + a_h^n\left(e_h^n, z_h\right) + \gamma_{\mathrm{s}} s_h(\mathcal{F}_{\Sigma_\delta^\pm}^n; e_h^n, z_h) = \mathcal{E}_I(z_h) + \mathcal{E}_0(z_h) + \mathcal{E}_\psi(z_h) + \mathcal{E}_\phi(z_h), \tag{10.53}$$

where

$$\mathcal{E}_I(z_h) := -\int_{\Omega_h^n} \frac{e^n - e^{n-1}}{\delta t} z_h d\boldsymbol{x} - a_h^n\left(e^n, z_h\right) - \gamma_{\mathrm{s}} s_h(\mathcal{F}_{\Sigma_\delta^\pm}^n; e^n, z_h). \tag{10.54}$$

Lemma 10.6. *Given $f \in L^q(\Omega_h^n)$, $g \in L^q(\Gamma_h^n)$, $w \in W^{1,p}(\mathcal{O}(\Omega_h^n))$, and $u \in W^{2,p}(\mathcal{O}(\Omega_h^n))$, where $\frac{1}{p} + \frac{1}{q} = 1$, there holds:*

$$\begin{aligned} \int_{\Omega_h^n} |(w \circ \boldsymbol{\Phi})f - wf|\, d\boldsymbol{x} &\lesssim h^{q+1} \|\nabla w\|_{L^p(\mathcal{O}(\Omega_h^n))} \|f\|_{L^q(\Omega_h^n)} \\ \int_{\Gamma_h^n} |(u \circ \boldsymbol{\Phi})g - ug|\, dS &\lesssim h^{q+1} \|u\|_{W^{2,p}(\mathcal{O}(\Omega_h^n))} \|g\|_{L^q(\Gamma_h^n)} \end{aligned} \tag{10.55}$$

Proof. We have

$$\begin{aligned} \int_{\Omega_h^n} |(w \circ \boldsymbol{\Phi})f - wf|\, d\boldsymbol{x} &= \int_{\Omega_h^n} \left| f \int_0^1 \nabla w(t\boldsymbol{\Phi} + (1-t)id) \cdot (\boldsymbol{\Phi} - id) \right| d\boldsymbol{x} \\ &\leq \|\boldsymbol{\Phi} - id\|_{L^\infty(\Omega_h^n)} \|\nabla w\|_{L^p(\mathcal{O}(\Omega_h^n))} \|f\|_{L^q(\Omega_h^n)} \\ &\lesssim h^{q+1} \|\nabla w\|_{L^p(\mathcal{O}(\Omega_h^n))} \|f\|_{L^q(\Omega_h^n)}, \end{aligned}$$

$$\begin{aligned} \int_{\Gamma_h^n} |(u \circ \boldsymbol{\Phi})g - ug|\, d\boldsymbol{x} &= \int_{\Gamma_h^n} \left| g \int_0^1 \nabla u(t\boldsymbol{\Phi} + (1-t)id) \cdot (\boldsymbol{\Phi} - id) \right| d\boldsymbol{x} \\ &\leq \|\boldsymbol{\Phi} - id\|_{L^\infty(\Gamma_h^n)} \|\nabla u\|_{W^{1,p}(\mathcal{O}(\Gamma_h^n))} \|g\|_{L^q(\Gamma_h^n)} \\ &\lesssim h^{q+1} \|u\|_{W^{2,p}(\mathcal{O}(\Omega_h^n))} \|g\|_{L^q(\Gamma_h^n)}. \end{aligned}$$

□

Lemma 10.7. *Given $f \in L^1(\Omega_h^n)$ and $g \in L^1(\Gamma_h^n)$, there holds:*

$$\begin{aligned} \left| \int_{\Omega_h^n} f \det(\nabla \boldsymbol{\Phi}) - f d\boldsymbol{x} \right| &\lesssim h^q |f\|_{L^1(\Omega_h^n)} \\ \left| \int_{\Gamma_h^n} g\mu_h - g d\boldsymbol{x} \right| &\lesssim h^q \|g\|_{L^1(\Gamma_h^n)} \end{aligned} \tag{10.56}$$

Proof. This proof follows from the basic properties of $\boldsymbol{\Phi}$. First, note

$$\begin{aligned} \left| \int_{\Omega_h^n} f[\det(\nabla \boldsymbol{\Phi}) - 1] d\boldsymbol{x} \right| &\leq \| \det(\nabla \boldsymbol{\Phi}) - 1\|_{L^\infty(\Omega_h^n)} \|f\|_{L^1(\Omega_h^n)} \\ &\lesssim h^q \|f\|_{L^1(\Omega_h^n)}, \end{aligned}$$

where we have used (4.31). Moreover, we have the following:

$$\begin{aligned} \left| \int_{\Gamma_h^n} g[\mu_h - 1] d\boldsymbol{x} \right| &\leq \|\mu_h - 1\|_{L^\infty(\Gamma_h^n)} \|g\|_{L^1(\Gamma_h^n)} \\ &\lesssim h^q \|g\|_{L^1(\Omega_h^n)}, \end{aligned}$$

where we have used (4.32). □

Lemma 10.8. *Given $\boldsymbol{v} \in [L^p(\Omega_h^n)]^d$, then we have the following:*

$$\|(\nabla \boldsymbol{\Phi}^T)^{-1} \boldsymbol{v} - \boldsymbol{v}\|_{L^p(\Omega_h^n)} \lesssim h^q \|\boldsymbol{v}\|_{L^p(\Omega_h^n)} \tag{10.57}$$

Proof. Note that $(\nabla \boldsymbol{\Phi}^T)^{-1} = (\nabla \boldsymbol{\Phi}^T - I + I)^{-1} = I + (\nabla \boldsymbol{\Phi}^T - I) + O(h^{2q}) \approx I + (\nabla \boldsymbol{\Phi}^T - I)$.

Thus, we get

$$\begin{aligned} \|(\nabla \boldsymbol{\Phi}^T)^{-1} \boldsymbol{v} - \boldsymbol{v}\|_{L^p(\Omega_h^n)}^p &= \int_{\Omega_h^n} \left| [(\nabla \boldsymbol{\Phi}^T)^{-1} - I] \boldsymbol{v} \right|^p d\boldsymbol{x} \\ &\lesssim \int_{\Omega_h^n} \left| (\nabla \boldsymbol{\Phi}^T - I) \boldsymbol{v} \right|^p d\boldsymbol{x} \\ &\leq \|\nabla \boldsymbol{\Phi} - I\|_{L^\infty(\Omega_h^n)}^p \|\boldsymbol{v}\|_{L^p(\Omega_h^n)}^p \\ &\lesssim h^{qp} \|\boldsymbol{v}\|_{L^p(\Omega_h^n)}^p. \end{aligned}$$

Hence, it follows that

$$\|(\nabla \boldsymbol{\Phi}^T)^{-1} \boldsymbol{v} - \boldsymbol{v}\|_{L^p(\Omega_h^n)} \lesssim h^q \|\boldsymbol{v}\|_{L^p(\Omega_h^n)}.$$

□

Lemma 10.9. *Assume the following regularity of the exact solution:*

$$y^n \in W^{2,\infty}(\mathcal{C}) \cap L^\infty([0,T]; H^{m+1}(\Omega(t))), \quad \partial_t y^n \in L^\infty([0,T]; H^m(\Omega(t))),$$

where $\mathcal{C} := \bigcup_{t\in(0,T)} \Omega(t) \times \{t\}$ *is the space-time cylinder. Then, we have the following estimate for* $\mathcal{E}_I(z_h)$*:*

$$|\mathcal{E}_I(z_h)| \lesssim h^m K^{1/2} \sup_{t\in[0,T]} \Big(\|y\|_{H^{m+1}(\Omega(t))} + \|y_t\|_{H^m(\Omega(t))}\Big) \cdot \Big[\|z_h\|_{H^1(\Omega_h^n)} + s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; z_h, z_h)^{1/2}\Big]$$

Proof. The proof follows from Lemma 5.12 in [50]. □

Lemma 10.10. *Assume* $y^n \in W^{2,\infty}(\mathcal{C}) \cap L^\infty([0,T]; H^{m+1}(\Omega(t)))$*. Then, we have the following estimate for* $\mathcal{E}_0(z_h)$*:*

$$|\mathcal{E}_0(z_h)| \lesssim [\delta t + h^q + h^m] \Bigg[\|y^n\|_{W^{2,\infty}(\mathcal{C})} + \sup_{t\in[0,T]} \|y\|_{H^{m+1}(\Omega(t))} + \sum_{n=1}^{N} \Big[\|f^n\|_{H^1(\Omega_h^n)} + \|g^n\|_{H^2(\Omega_h^n)}\Big]\Bigg] \cdot \\ \cdot \Big[\|z_h\|_{H^1(\Omega_h^n)} + s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; z_h, z_h)^{1/2}\Big]. \tag{10.58}$$

Proof. For $\mathcal{E}_1(z_h)$ we use Taylor's Theorem using the integral form of the remainder:

$$y(\boldsymbol{x}, t_{n-1}) = y(\boldsymbol{x}, t_n) + y_t(\boldsymbol{x}, t_n)(t_{n-1} - t_n) + \int_{t_n}^{t_{n-1}} y_{tt}(\boldsymbol{x}, t)(t_{n-1} - t)dt.$$

Then, we get the following:

$$\begin{aligned} \mathcal{E}_1(z_h) &= \int_{\Omega_h^n} \frac{y^n - y^{n-1}}{\delta t} z_h d\boldsymbol{x} - \int_{\Omega^n} y_t^n z_h^\ell d\boldsymbol{x} \\ &= \int_{\Omega_h^n} y_t(\boldsymbol{x}, t_n) z_h + \int_{t_{n-1}}^{t_n} \frac{y_{tt}(\boldsymbol{x}, t)}{\delta t}(t_{n-1} - t) z_h dt d\boldsymbol{x} - \int_{\Omega^n} y_t^n z_h^\ell d\boldsymbol{x} \\ &= \int_{\Omega_h^n} \int_{t_{n-1}}^{t_n} \frac{y_{tt}(\boldsymbol{x}, t)}{\delta t}(t_{n-1} - t) dt z_h d\boldsymbol{x} + \int_{\Omega_h^n} y_t(\boldsymbol{x}, t_n) z_h d\boldsymbol{x} - \int_{\Omega^n} y_t^n z_h^\ell d\boldsymbol{x} \\ &= \int_{\Omega_h^n} \int_{t_{n-1}}^{t_n} \frac{y_{tt}(\boldsymbol{x}, t)}{\delta t}(t_{n-1} - t) dt z_h d\boldsymbol{x} + \int_{\Omega_h^n} y_t(\boldsymbol{x}, t_n) z_h d\boldsymbol{x} - \int_{\Omega_h^n} (y_t^n \circ \boldsymbol{\Phi}) z_h \det(\nabla \boldsymbol{\Phi}) d\boldsymbol{x}, \end{aligned} \tag{10.59}$$

where in the last line we performed a change of variables. And now we split the above into two parts:

$$
\begin{aligned}
\left|\int_{\Omega_h^n}\int_{t_{n-1}}^{t_n}\frac{y_{tt}(\boldsymbol{x},t)}{\delta t}(t_{n-1}-t)dtz_h d\boldsymbol{x}\right| &\leq \frac{1}{\delta t}\|y_{tt}\|_{L^\infty(\mathcal{O}(Q))}\int_{t_{n-1}}^{t_n}|t_{n-1}-t|dt\int_{\Omega_h^n}|z_h|d\boldsymbol{x}\\
&= \frac{1}{\delta t}\|y_{tt}\|_{L^\infty(\mathcal{O}(Q))}\frac{1}{2}\delta t^2\|z_h\|_{L^1(\Omega_h^n)}\\
&\lesssim \delta t\|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{L^2(\Omega_h^n)},
\end{aligned} \tag{10.60}
$$

where we have used Hölder's inequality and some standard techniques. Next,

$$
\begin{aligned}
&\left|\int_{\Omega_h^n} y_t(\boldsymbol{x},t_n)z_h d\boldsymbol{x}-\int_{\Omega_h^n}(y_t^n\circ\boldsymbol{\Phi})z_h\det(\nabla\boldsymbol{\Phi})d\boldsymbol{x}\right|\\
\leq&\left|\int_{\Omega_h^n} y_t^n z_h-(y_t^n\circ\boldsymbol{\Phi})z_h d\boldsymbol{x}\right|+h^q\int_{\Omega_h^n}|(y_t^n\circ\boldsymbol{\Phi})z_h|d\boldsymbol{x}\\
\lesssim& h^{q+1}\left\|\nabla y_t^n\right\|_{L^\infty(\mathcal{O}(\Omega_h^n))}\left\|z_h\right\|_{L^1(\Omega_h^n)}+h^q\|y_t^n\|_{L^\infty(\mathcal{O}(\Omega_h^n))}\|z_h\|_{L^1(\Omega_h^n)}\\
\lesssim& h^q\|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{L^2(\Omega_h^n)},
\end{aligned} \tag{10.61}
$$

where we have used the fundamental theorem of calculus for line integrals, Corollary 4.13, the geometry approximation between the discrete and exact domains, and some other standard estimates.

Now we handle $\mathcal{E}_2(z_h)$:

$$
|\mathcal{E}_2(z_h)| = \left|a_h^n\left(y^n,z_h\right)-a^n\left(y^n,z_h^\ell\right)\right|, \tag{10.62}
$$

and we recall the definitions of $a_h^n\left(\cdot,\cdot\right)$ and $a^n\left(\cdot,\cdot\right)$.

$$
\begin{aligned}
a_h^n\left(y^n,z_h\right) &= \frac{1}{2}\int_{\Omega_h^n}(\mathbf{v}\cdot\nabla y^n)z_h-(\mathbf{v}\cdot\nabla z_h)y^n d\boldsymbol{x}+\int_{\Omega_h^n}(A\nabla y^n)\cdot\nabla z_h d\boldsymbol{x}\\
&\quad+\frac{1}{2}\int_{\Gamma_h^n}(\boldsymbol{\nu}\cdot\mathbf{v})y^n z_h dS+\int_{\Gamma_h^n} w_0 y^n z_h dS,\\
a^n\left(y^n,z_h^\ell\right) &= \frac{1}{2}\int_{\Omega^n}(\mathbf{v}\cdot\nabla y^n)z_h^\ell-(\mathbf{v}\cdot\nabla z_h^\ell)y^n d\boldsymbol{x}+\int_{\Omega^n}(A\nabla y^n)\cdot\nabla z_h^\ell d\boldsymbol{x}\\
&\quad+\frac{1}{2}\int_{\Gamma^n}(\boldsymbol{\nu}\cdot\mathbf{v})y^n z_h^\ell dS+\int_{\Gamma^n} w_0 y^n z_h^\ell dS.
\end{aligned}
$$

Next, we split (10.62) using the triangle inequality:

$$
\begin{aligned}
|\mathcal{E}_2(z_h)| &\le I_1 + I_2 + I_3 + I_4 + I_5, \\
I_1 &:= \left| \int_{\Omega_h^n} (\mathbf{v} \cdot \nabla y^n) z_h d\boldsymbol{x} - \int_{\Omega^n} (\mathbf{v} \cdot \nabla y^n) z_h^\ell d\boldsymbol{x} \right|, \\
I_2 &:= \left| \int_{\Omega_h^n} (\mathbf{v} \cdot \nabla z_h) y^n d\boldsymbol{x} - \int_{\Omega^n} (\mathbf{v} \cdot \nabla z_h^\ell) y^n d\boldsymbol{x} \right|, \\
I_3 &:= \left| \int_{\Omega_h^n} (A \nabla y^n) \cdot \nabla z_h d\boldsymbol{x} - \int_{\Omega^n} (A \nabla y^n) \cdot \nabla z_h^\ell d\boldsymbol{x} \right|, \\
I_4 &:= \left| \int_{\Gamma_h^n} (\boldsymbol{\nu} \cdot \mathbf{v}) y^n z_h dS - \int_{\Gamma^n} (\boldsymbol{\nu} \cdot \mathbf{v}) y^n z_h^\ell dS \right|, \\
I_5 &:= \left| \int_{\Gamma_h^n} w_0 y^n z_h dS - \int_{\Gamma^n} w_0 y^n z_h^\ell dS \right|,
\end{aligned}
$$

and we deal with the terms one by one. First,

$$
\begin{aligned}
I_1 &= \left| \int_{\Omega_h^n} (\mathbf{v} \cdot \nabla y^n) z_h d\boldsymbol{x} - \int_{\Omega^n} (\mathbf{v} \cdot \nabla y^n) z_h^\ell d\boldsymbol{x} \right| \\
&= \left| \int_{\Omega_h^n} (\mathbf{v} \cdot \nabla y^n) z_h - [(\mathbf{v} \cdot \nabla y^n) \circ \mathbf{\Phi}] z_h \det(\nabla \mathbf{\Phi}) d\boldsymbol{x} \right| \\
&\lesssim \left| \int_{\Omega_h^n} (\mathbf{v} \cdot \nabla y^n) z_h - [(\mathbf{v} \cdot \nabla y^n) \circ \mathbf{\Phi}] z_h d\boldsymbol{x} \right| + h^q \|[(\mathbf{v} \cdot \nabla y^n) \circ \mathbf{\Phi}] z_h\|_{L^1(\Omega_h^n)} \\
&\lesssim h^{q+1} \|\nabla(\mathbf{v} \cdot \nabla y^n)\|_{L^\infty(\mathcal{O}(\Omega_h^n))} \|z_h\|_{L^1(\Omega_h^n)} + h^q \|\mathbf{v}\|_{L^\infty(\Omega^n)} \|\nabla y^n\|_{L^\infty(\Omega^n)} \|z_h\|_{L^1(\Omega_h^n)} \\
&\lesssim h^{q+1} \|(\nabla \mathbf{v}) \nabla y^n + (\nabla^2 y^n) \mathbf{v}\|_{L^\infty(\mathcal{O}(\Omega_h^n))} \|z_h\|_{L^2(\Omega_h^n)} + h^q \|\mathbf{v}\|_{L^\infty(\Omega^n)} \|y\|_{W^{2,\infty}(\mathcal{C})} \|z_h\|_{L^2(\Omega_h^n)} \\
&\lesssim h^{q+1} \|\mathbf{v}\|_{W^{1,\infty}(\mathcal{O}(\Omega_h^n))} \|y\|_{W^{2,\infty}(\mathcal{O}(Q))} \|z_h\|_{L^2(\Omega_h^n)} + h^q \|\mathbf{v}\|_{L^\infty(\Omega^n)} \|y\|_{W^{2,\infty}(\mathcal{C})} \|z_h\|_{L^2(\Omega_h^n)} \\
&\lesssim h^q \|y\|_{W^{2,\infty}(\mathcal{C})} \|z_h\|_{L^2(\Omega_h^n)},
\end{aligned}
\tag{10.63}
$$

where we have used a basic change of variables and Lemmas 10.6 and 10.7. Next,

$$
\begin{aligned}
I_2 &= \left| \int_{\Omega_h^n} (\mathbf{v} \cdot \nabla z_h) y^n d\boldsymbol{x} - \int_{\Omega^n} (\mathbf{v} \cdot \nabla z_h^\ell) y^n d\boldsymbol{x} \right| \\
&= \left| \int_{\Omega_h^n} (y^n \mathbf{v} \cdot \nabla z_h) - [(y^n \mathbf{v} \cdot \nabla z_h^\ell) \circ \boldsymbol{\Phi}] \det(\nabla \boldsymbol{\Phi}) d\boldsymbol{x} \right| \\
&\lesssim \left| \int_{\Omega_h^n} (y^n \mathbf{v} \cdot \nabla z_h) - [(y^n \mathbf{v}) \circ \boldsymbol{\Phi}] \cdot (\nabla z_h^\ell \circ \boldsymbol{\Phi}) d\boldsymbol{x} \right| + h^q \left\| (y^n \mathbf{v} \cdot \nabla z_h^\ell) \circ \boldsymbol{\Phi} \right\|_{L^1(\Omega_h^n)} \\
&\lesssim \left| \int_{\Omega_h^n} (y^n \mathbf{v} \cdot \nabla z_h) - [(y^n \mathbf{v}) \circ \boldsymbol{\Phi}] \cdot (\nabla \boldsymbol{\Phi})^{-1} \nabla z_h d\boldsymbol{x} \right| + h^q \|\mathbf{v}\|_{L^\infty(\Omega^n)} \|y^n\|_{L^\infty(\Omega^n)} \|\nabla z_h^\ell \circ \boldsymbol{\Phi}\|_{L^2(\Omega_h^n)} \\
&\lesssim \left| \int_{\Omega_h^n} (y^n \mathbf{v} - (y^n \mathbf{v}) \circ \boldsymbol{\Phi}) \cdot \nabla z_h d\boldsymbol{x} \right| + h^q \int_{\Omega_h^n} |[(y^n \mathbf{v}) \circ \boldsymbol{\Phi}] \cdot \nabla z_h| d\boldsymbol{x} \\
&\qquad + h^q \|\mathbf{v}\|_{L^\infty(\Omega^n)} \|y\|_{W^{2,\infty}(\mathcal{C})} \|(\nabla \boldsymbol{\Phi})^{-1} \nabla z_h\|_{L^2(\Omega_h^n)} \\
&\lesssim h^{q+1} \|\nabla (y^n \mathbf{v})\|_{L^\infty(\mathcal{O}(\Omega_h^n))} \|\nabla z_h\|_{L^1(\Omega_h^n)} + h^q \|\mathbf{v}\|_{L^\infty(\Omega^n)} \|y^n\|_{L^\infty(\Omega^n)} \|\nabla z_h\|_{L^1(\Omega_h^n)} \\
&\qquad + h^q \|\mathbf{v}\|_{L^\infty(\Omega^n)} \|y\|_{W^{2,\infty}(\mathcal{C})} \|\nabla z_h\|_{L^2(\Omega_h^n)} + h^{2q} \|\mathbf{v}\|_{L^\infty(\Omega^n)} \|y\|_{W^{2,\infty}(\mathcal{C})} \|\nabla z_h\|_{L^2(\Omega_h^n)} \\
&\lesssim h^q \|\nabla y^n (\mathbf{v})^T + y^n \nabla \mathbf{v}\|_{L^\infty(\mathcal{O}(\Omega_h^n))} \|z_h\|_{H^1(\Omega_h^n)} + h^q \|y\|_{W^{2,\infty}(\mathcal{C})} \|z_h\|_{H^1(\Omega_h^n)} \\
&\lesssim h^q \|y\|_{W^{2,\infty}(\mathcal{C})} \|z_h\|_{H^1(\Omega_h^n)},
\end{aligned}
\tag{10.64}
$$

where, again we have used a basic change of variables and Lemmas 10.6, 10.7, and 10.8.

For I_3, we have

$$
\begin{aligned}
I_3 &= \left|\int_{\Omega_h^n} (A\nabla y^n)\cdot \nabla z_h d\boldsymbol{x} - \int_{\Omega^n} (A\nabla y^n)\cdot \nabla z_h^\ell d\boldsymbol{x}\right| \\
&= \left|\int_{\Omega_h^n} (A\nabla y^n)\cdot \nabla z_h - (A(\nabla y^n\circ \boldsymbol{\Phi}))\cdot(\nabla z_h^\ell)\circ \boldsymbol{\Phi} \det(\nabla \boldsymbol{\Phi}) d\boldsymbol{x}\right| \\
&\lesssim \left|\int_{\Omega_h^n} (A\nabla y^n)\cdot \nabla z_h - (A(\nabla y^n\circ \boldsymbol{\Phi}))\cdot(\nabla z_h^\ell)\circ \boldsymbol{\Phi} d\boldsymbol{x}\right| + h^q \|(A(\nabla y^n\circ\boldsymbol{\Phi}))\cdot(\nabla z_h^\ell)\circ\boldsymbol{\Phi}\|_{L^1(\Omega_h^n)} \\
&\lesssim \left|\int_{\Omega_h^n} (A\nabla y^n)\cdot \nabla z_h - (A(\nabla y^n\circ \boldsymbol{\Phi}))\cdot(\nabla \boldsymbol{\Phi})^{-1}\nabla z_h d\boldsymbol{x}\right| + h^q\|A\|_\infty \|\nabla y^n\|_{L^\infty(\Omega^n)} \|(\nabla\boldsymbol{\Phi})^{-1}\nabla z_h\|_{L^1(\Omega_h^n)} \\
&\lesssim \left|\int_{\Omega_h^n} (A\nabla y^n)\cdot \nabla z_h - (A(\nabla y^n\circ \boldsymbol{\Phi}))\cdot \nabla z_h d\boldsymbol{x}\right| + h^q\|A\|_\infty \|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{H^1(\Omega_h^n)} \\
&\lesssim h^{q+1}\|\nabla(A\nabla y^n)\|_{L^\infty(\mathcal{O}(\Omega_h^n))}\|\nabla z_h\|_{L^1(\Omega_h^n)} + h^q\|A\|_\infty\|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{H^1(\Omega_h^n)} \\
&\lesssim h^{q+1}\|A\|_\infty\|\nabla^2 y^n\|_{L^\infty(\Omega_h^n)}\|z_h\|_{H^1(\Omega_h^n)} + h^q\|A\|_\infty\|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{H^1(\Omega_h^n)} \\
&\lesssim h^q\|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{H^1(\Omega_h^n)},
\end{aligned} \tag{10.65}
$$

where we, again used a basic change of variables and Lemmas 10.6, 10.7, and 10.8. Then,

$$
\begin{aligned}
I_4 &= \left|\int_{\Gamma_h^n} (\boldsymbol{\nu}\cdot \mathbf{v}) y^n z_h dS - \int_{\Gamma^n} (\boldsymbol{\nu}\cdot\mathbf{v}) y^n z_h^\ell dS\right| \\
&= \left|\int_{\Gamma_h^n} (\boldsymbol{\nu}\cdot \mathbf{v}) y^n z_h - \boldsymbol{\nu}\cdot((y^n\mathbf{v})\circ\boldsymbol{\Phi}) z_h \mu_h dS\right| \\
&\lesssim \left|\int_{\Gamma_h^n} (\boldsymbol{\nu}\cdot \mathbf{v}) y^n z_h - \boldsymbol{\nu}\cdot((y^n\mathbf{v})\circ\boldsymbol{\Phi}) z_h dS\right| + h^q\|(\boldsymbol{\nu}\cdot(\mathbf{v}\circ\boldsymbol{\Phi}))(y^n\circ\boldsymbol{\Phi})z_h\|_{L^1(\Gamma_h^n)} \\
&\lesssim h^{q+1}\|\nabla(y^n\mathbf{v})\|_{L^\infty(\mathcal{O}(\Omega_h^n))}\|z_h\|_{L^1(\Gamma_h^n)} + h^q\|\mathbf{v}\|_{L^\infty(\Gamma^n)}\|y^n\|_{L^\infty(\Gamma^n)}\|z_h\|_{L^1(\Gamma_h^n)} \\
&\lesssim h^{q+1}\|\nabla y^n \mathbf{v}^T + y^n\nabla\mathbf{v}\|_{L^\infty(\Omega_h^n)}\|z_h\|_{H^1(\Omega_h^n)} + h^q\|\mathbf{v}\|_{L^\infty(\Gamma^n)}\|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{H^1(\Omega_h^n)} \\
&\lesssim h^q\|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{H^1(\Omega_h^n)}.
\end{aligned}
$$

The term $I_5 = \left|\int_{\Gamma_h^n} w_0 y^n z_h dS - \int_{\Gamma^n} w_0 y^n z_h^\ell dS\right| \lesssim h^q\|y\|_{W^{2,\infty}(\mathcal{C})}\|z_h\|_{H^1(\Omega_h^n)}$ is handled in the same way as the previous term except it is a little simpler since there is no need to deal with the material velocity. And now putting everything together we get the following:

$$|\mathcal{E}_2(z_h)| \lesssim h^q \|y\|_{W^{2,\infty}(\mathcal{C})} \|z_h\|_{H^1(\Omega_h^n)}.$$

Now, we handle $\mathcal{E}_3(z_h)$ using a Cauchy-Schwarz inequality and Proposition (4.4):

$$\begin{aligned}|\mathcal{E}_3(z_h)| &= |\gamma_{\mathrm{s}} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; y^n, z_h)| \\ &\leq \gamma_{\mathrm{s}} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; y^n, y^n)^{1/2} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; z_h, z_h)^{1/2} \\ &\lesssim h^m \|y\|_{H^{m+1}(\mathcal{O}_\delta(\Omega_h^n))} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; z_h, z_h)^{1/2} \\ &\lesssim h^m \|y\|_{H^{m+1}(\Omega^n)} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; z_h, z_h)^{1/2}.\end{aligned} \tag{10.66}$$

Next, we estimate $\mathcal{E}_4(z_h)$:

$$\begin{aligned}|\mathcal{E}_4(z_h)| &= \left|\chi^n\left(z_h^\ell\right) - \chi_h^n\left(z_h\right)\right| \\ &= \left|\int_{\Omega^n} f^n z_h^\ell d\boldsymbol{x} + \int_{\Gamma^n} (g^n + w_0 y_\Gamma^n) z_h^\ell dS - \int_{\Omega_h^n} f_h^n z_h d\boldsymbol{x} - \int_{\Gamma_h^n} (g_h^n + w_0 y_{\Gamma,h}^n) z_h dS\right| \\ &= \left|\int_{\Omega_h^n} (f^n \circ \boldsymbol{\Phi}) z_h \det(\nabla\boldsymbol{\Phi}) - f_h^n z_h d\boldsymbol{x} + \int_{\Gamma_h^n} ((g^n + w_0 y_\Gamma^n) \circ \boldsymbol{\Phi}) z_h \mu_h - (g_h^n + w_0 y_{\Gamma,h}^n) z_h dS\right| \\ &\leq \left|\int_{\Omega_h^n} (f^n \circ \boldsymbol{\Phi}) z_h \det(\nabla\boldsymbol{\Phi}) - f_h^n z_h d\boldsymbol{x}\right| \\ &\qquad + \left|\int_{\Gamma_h^n} ((g^n + w_0 y_\Gamma^n) \circ \boldsymbol{\Phi}) z_h \mu_h - (g_h^n + w_0 y_{\Gamma,h}^n) z_h dS\right|,\end{aligned} \tag{10.67}$$

where all we have done so far is use a change of variables. Then, we deal with the two terms separately:

$$
\begin{aligned}
&\left|\int_{\Omega_h^n}(f^n\circ\boldsymbol{\Phi})z_h\det(\nabla\boldsymbol{\Phi})-f_h^n z_h d\boldsymbol{x}\right|\\
\lesssim&\left|\int_{\Omega_h^n}(f^n\circ\boldsymbol{\Phi})z_h-f^n z_h d\boldsymbol{x}\right|+h^q\int_{\Omega_h^n}|(f^n\circ\boldsymbol{\Phi})z_h|\,d\boldsymbol{x}\\
\lesssim& h^{q+1}\|\nabla f^n\|_{L^2(\mathcal{O}(\Omega_h^n))}\|z_h\|_{L^2(\Omega_h^n)}+h^q\|f^n\circ\boldsymbol{\Phi}\|_{L^2(\Omega_h^n)}\|z_h\|_{L^2(\Omega_h^n)}\\
\lesssim& h^{q+1}\|f^n\|_{H^1(\mathcal{O}(\Omega_h^n))}\|z_h\|_{L^2(\Omega_h^n)}+h^q\|f^n\|_{L^2(\Omega^n)}\|z_h\|_{L^2(\Omega_h^n)}\\
\lesssim& h^q\|f^n\|_{H^1(\mathcal{O}(\Omega_h^n))}\|z_h\|_{L^2(\Omega_h^n)},
\end{aligned}
\tag{10.68}
$$

$$
\begin{aligned}
&\left|\int_{\Gamma_h^n}((g^n+w_0y_\Gamma^n)\circ\boldsymbol{\Phi})z_h\mu_h-(g_h^n+w_0y_{\Gamma,h}^n)z_h dS\right|\\
\lesssim&\left|\int_{\Gamma_h^n}((g^n+w_0y_\Gamma^n)\circ\boldsymbol{\Phi})z_h-(g^n+w_0y_\Gamma^n)z_h dS\right|+h^q\int_{\Gamma_h^n}|((g^n+w_0y_\Gamma^n)\circ\boldsymbol{\Phi})z_h|\,dS\\
\lesssim&\left|\int_{\Gamma_h^n}\nabla g^n(t\boldsymbol{\Phi}+(1-t)id)\cdot(\boldsymbol{\Phi}-id)z_h dS\right|+h^q\|g^n\circ\boldsymbol{\Phi}\|_{H^1(\Omega_h^n)}\|z_h\|_{H^1(\Omega_h^n)}\\
\lesssim& h^{q+1}\|g^n\|_{H^2(\mathcal{O}(\Omega_h^n))}\|z_h\|_{H^1(\Omega_h^n)}+h^q\|g^n\|_{H^1(\Omega_h^n)}\|z_h\|_{H^1(\Omega_h^n)}\\
\lesssim& h^q\|g^n\|_{H^2(\mathcal{O}(\Omega_h^n))}\|z_h\|_{H^1(\Omega_h^n)}.
\end{aligned}
\tag{10.69}
$$

Hence, it follows that

$$
\begin{aligned}
|\mathcal{E}_4(z_h)|&\lesssim h^q\|f^n\|_{H^1(\mathcal{O}(\Omega_h^n))}\|z_h\|_{L^2(\Omega_h^n)}+h^q\|g^n\|_{H^2(\mathcal{O}(\Omega_h^n))}\|z_h\|_{H^1(\Omega_h^n)}\\
&\lesssim h^q\left[\|f^n\|_{H^1(\Omega_h^n)}+\|g^n\|_{H^2(\Omega_h^n)}\right]\|z_h\|_{H^1(\Omega_h^n)}.
\end{aligned}
$$

Combining the estimates for $\mathcal{E}_i(z_h)$ with $i=1,2,3,4$, the proof is finished. □

Lemma 10.11. *Assume $y^n \in H^{m+1}(\Omega)$ for $m \geq 1$. Then, we have the following estimate:*

$$
\begin{aligned}
|\mathcal{E}_{\psi_c}(z_h)| &:= \left| \int_{\Omega_h^n} \psi_c'(y_h^n) z_h d\boldsymbol{x} - \int_{\Omega^n} \psi_c'(y^n) z_h^\ell d\boldsymbol{x} \right| \\
&\lesssim \left[h^q + h^{m+1}\right] \left[\|y^n\|^3_{H^{m+1}(\Omega_h^n)} + C\right] \|z_h\|_{H^1(\Omega_h^n)} \\
&\quad + \left[\|y_h^n\|^2_{H^1(\Omega_h^n)} + \|y^n\|^2_{H^1(\Omega_h^n)} + C\right] \|e_h^n\|_{L^2(\Omega_h^n)} \|z_h\|_{H^1(\Omega_h^n)}, \\
\left|\mathcal{E}_{\psi_e}(e_h^n) + \int_{\Omega_h^n} \psi_e'(e_h^n) e_h^n d\boldsymbol{x}\right| &:= \left| \int_{\Omega_h^n} \psi_e'(y_h^n) z_h d\boldsymbol{x} - \int_{\Omega^n} \psi_e'(y^n) z_h^\ell d\boldsymbol{x} + \int_{\Omega_h^n} \psi_e'(e_h^n) e_h^n d\boldsymbol{x} \right| \\
&\lesssim \left[h^q + h^{m+1}\right] \|y^n\|_{H^{m+1}(\Omega_h^n)} \|e_h^n\|_{L^2(\Omega_h^n)}.
\end{aligned}
\tag{10.70}
$$

This results in the following estimate:

$$
\begin{aligned}
\left|\mathcal{E}_{\psi}(e_h^n) + \int_{\Omega_h^n} \psi_e'(e_h^n) e_h^n d\boldsymbol{x}\right| &\lesssim \left[h^q + h^{m+1}\right] \left[\|y^n\|^3_{H^{m+1}(\Omega_h^n)} + C\right] \|e_h^n\|_{H^1(\Omega_h^n)} \\
&\quad + \left[\|y_h^n\|^2_{H^1(\Omega_h^n)} + \|y^n\|^2_{H^1(\Omega_h^n)} + C\right] \|e_h^n\|_{L^2(\Omega_h^n)} \|e_h^n\|_{H^1(\Omega_h^n)}
\end{aligned}
\tag{10.71}
$$

Proof. Using a change of variables, we have the following:

$$
\int_{\Omega^n} \psi_c'(y^n) z_h^\ell d\boldsymbol{x} = \int_{\Omega_h^n} \psi_c'(y^n \circ \mathbf{\Phi}) z_h \det(\nabla \mathbf{\Phi}) d\boldsymbol{x}.
$$

Now using the fundamental theorem of calculus for line integrals and some standard techniques we get

$$
\begin{aligned}
&|\mathcal{E}_{\psi_c}(z_h)| \\
=& \left| \int_{\Omega_h^n} \psi_c'(y_h^n) z_h d\boldsymbol{x} - \int_{\Omega^n} \psi_c'(y^n) z_h^\ell d\boldsymbol{x} \right| \\
=& \left| \int_{\Omega_h^n} \psi_c'(y_h^n) z_h d\boldsymbol{x} - \int_{\Omega_h^n} \psi_c'(y^n \circ \boldsymbol{\Phi}) z_h \det(\nabla \boldsymbol{\Phi}) d\boldsymbol{x} \right| \\
\leq& \left| \int_{\Omega_h^n} \psi_c'(y^n \circ \boldsymbol{\Phi}) z_h \left[\det(\nabla \boldsymbol{\Phi}) - 1\right] d\boldsymbol{x} \right| + \left| \int_{\Omega_h^n} \left[\psi_c'(y_h^n) - \psi_c'(y^n \circ \boldsymbol{\Phi})\right] z_h d\boldsymbol{x} \right| \\
\lesssim& h^q \int_{\Omega_h^n} |\psi_c'(y^n \circ \boldsymbol{\Phi}) z_h| \, d\boldsymbol{x} + \left| \int_{\Omega_h^n} \left[\psi_c'(y^n) - \psi_c'(y^n \circ \boldsymbol{\Phi})\right] z_h d\boldsymbol{x} \right| + \left| \int_{\Omega_h^n} \left[\psi_c'(y_h^n) - \psi_c'(y^n)\right] z_h d\boldsymbol{x} \right| \\
\lesssim& h^q \int_{\Omega_h^n} |\psi_c'(y^n \circ \boldsymbol{\Phi}) z_h| \, d\boldsymbol{x} + \left| \int_{\Omega_h^n} \psi_c''(c_1 y^n + (1 - c_1)(y^n \circ \boldsymbol{\Phi})) \cdot (y^n - y^n \circ \boldsymbol{\Phi}) z_h d\boldsymbol{x} \right| \\
&\qquad + \left| \int_{\Omega_h^n} \psi_c''(c_2 y_h^n + (1 - c_2) y^n) \cdot (y_h^n - y^n) z_h d\boldsymbol{x} \right|,
\end{aligned}
\tag{10.72}
$$

where we have used the geometry approximation and the mean value theorem with $c_1, c_2 \in [0, 1]$. And now we use Hölder's inequality on all three terms. Due to the Sobolev embedding theorems we have that $z_h \in H^1(\Omega_h^n) \implies z_h \in L^6(\Omega_h^n)$ for $\Omega_h^n \subset \mathbb{R}^3$. Hence,

$$
\begin{aligned}
&|\mathcal{E}_{\psi_c}(z_h)| \\
\lesssim & h^q \|\psi_c'(y^n \circ \mathbf{\Phi})\|_{L^2(\Omega_h^n)} \|z_h\|_{L^2(\Omega_h^n)} \\
&\quad + \|\psi_c''(c_1 y^n + (1-c_1)(y^n \circ \mathbf{\Phi}))\|_{L^3(\Omega_h^n)} \|y^n - y^n \circ \mathbf{\Phi}\|_{L^2(\Omega_h^n)} \|z_h\|_{L^6(\Omega_h^n)} \\
&\quad + \|\psi_c''(c_2 y_h^n + (1-c_2)y^n)\|_{L^3(\Omega_h^n)} \|y_h^n - y^n\|_{L^2(\Omega_h^n)} \|z_h\|_{L^6(\Omega_h^n)} \\
\lesssim & h^q \left[\|y^n \circ \mathbf{\Phi}\|_{L^6(\Omega_h^n)}^3 + C \right] \|z_h\|_{L^2(\Omega_h^n)} \\
&\quad + h^{q+1} \left\| (y^n)^2 + (y^n \circ \mathbf{\Phi})^2 + C \right\|_{L^3(\Omega_h^n)} \|\nabla y^n\|_{L^2(\Omega_h^n)} \|z_h\|_{L^6(\Omega_h^n)} \\
&\quad + \left\| (y_h^n)^2 + (y^n)^2 + C \right\|_{L^3(\Omega_h^n)} \|\mathbb{E}^n\|_{L^2(\Omega_h^n)} \|z_h\|_{L^6(\Omega_h^n)} \\
\lesssim & h^q \left[\|y^n\|_{L^6(\Omega_h^n)}^3 + C \right] \|z_h\|_{L^2(\Omega_h^n)} \\
&\quad + h^{q+1} \left[\|y^n\|_{L^6(\Omega_h^n)}^2 + C \right] \|y^n\|_{H^1(\Omega_h^n)} \|z_h\|_{L^6(\Omega_h^n)} \\
&\quad + \left[\|y_h^n\|_{L^6(\Omega_h^n)}^2 + \|y^n\|_{L^6(\Omega_h^n)}^2 + C \right] \left[\|e_h^n\|_{L^2(\Omega_h^n)} + \|e^n\|_{L^2(\Omega_h^n)} \right] \|z_h\|_{L^6(\Omega_h^n)} \\
\lesssim & h^q \left[\|y^n\|_{H^1(\Omega_h^n)}^3 + C \right] \|z_h\|_{L^2(\Omega_h^n)} \\
&\quad + h^{q+1} \left[\|y^n\|_{H^1(\Omega_h^n)}^3 + C \right] \|z_h\|_{H^1(\Omega_h^n)} \\
&\quad + \left[\|y_h^n\|_{H^1(\Omega_h^n)}^2 + \|y^n\|_{H^1(\Omega_h^n)}^2 + C \right] \left[\|e_h^n\|_{L^2(\Omega_h^n)} + h^{m+1} \|y^n\|_{H^{m+1}(\Omega_h^n)} \right] \|z_h\|_{H^1(\Omega_h^n)} \\
\lesssim & \left[h^q + h^{m+1} \right] \left[\|y^n\|_{H^{m+1}(\Omega_h^n)}^3 + C \right] \|z_h\|_{H^1(\Omega_h^n)} \\
&\quad + \left[\|y_h^n\|_{H^1(\Omega_h^n)}^2 + \|y^n\|_{H^1(\Omega_h^n)}^2 + C \right] \|e_h^n\|_{L^2(\Omega_h^n)} \|z_h\|_{H^1(\Omega_h^n)},
\end{aligned}
\tag{10.73}
$$

where in the last few lines we used Young's inequality, the fact that ψ_c is a quartic polynomial, the geometry approximation between Ω^n and Ω_h^n, and Corollary 4.13. For the other inequality, we have

$$
\begin{aligned}
&\left|\mathcal{E}_{\psi_e}(e_h^n) + \int_{\Omega_h^n} \psi_e'(e_h^n) e_h^n d\boldsymbol{x}\right| \\
=&\left|\int_{\Omega_h^n} \psi_e'(y_h^n) e_h^n d\boldsymbol{x} - \int_{\Omega^n} \psi_e'(y^n)(e_h^n)^\ell d\boldsymbol{x} + \int_{\Omega_h^n} \psi_e'(e_h^n) e_h^n d\boldsymbol{x}\right| \\
=&\left|\int_{\Omega_h^n} \psi_e'(y_h^n) e_h^n - \psi_e'(y^n \circ \boldsymbol{\Phi}) e_h^n \det(\nabla \boldsymbol{\Phi}) d\boldsymbol{x} + \int_{\Omega_h^n} \psi_e'(e_h^n) e_h^n d\boldsymbol{x}\right| \\
\leq&\left|\int_{\Omega_h^n} \psi_e'(y^n \circ \boldsymbol{\Phi}) e_h^n \left[\det(\nabla \boldsymbol{\Phi}) - 1\right] d\boldsymbol{x}\right| + \left|\int_{\Omega_h^n} \left[\psi_e'(y_h^n) - \psi_e'(y^n \circ \boldsymbol{\Phi}) + \psi_e'(e_h^n)\right] e_h^n d\boldsymbol{x}\right| \\
\lesssim& h^q \int_{\Omega_h^n} \left|\psi_e'(y^n \circ \boldsymbol{\Phi}) e_h^n\right| d\boldsymbol{x} + \left|\int_{\Omega_h^n} \left[\psi_e'(y_I^n) - \psi_e'(y^n \circ \boldsymbol{\Phi})\right] e_h^n d\boldsymbol{x}\right| \\
\lesssim& h^q \int_{\Omega_h^n} \left|\psi_e'(y^n \circ \boldsymbol{\Phi}) e_h^n\right| d\boldsymbol{x} + \left|\int_{\Omega_h^n} \left[\psi_e'(y^n) - \psi_e'(y^n \circ \boldsymbol{\Phi})\right] e_h^n d\boldsymbol{x}\right| + \left|\int_{\Omega_h^n} \left[\psi_e'(y_I^n) - \psi_e'(y^n)\right] e_h^n d\boldsymbol{x}\right| \\
\lesssim& h^q \int_{\Omega_h^n} \left|\psi_e'(y^n \circ \boldsymbol{\Phi}) e_h^n\right| d\boldsymbol{x} + \left|\int_{\Omega_h^n} \beta_\psi (y^n - y^n \circ \boldsymbol{\Phi}) e_h^n d\boldsymbol{x}\right| + \left|\int_{\Omega_h^n} \psi_e'(e^n) e_h^n d\boldsymbol{x}\right|,
\end{aligned}
\tag{10.74}
$$

where we have used the fact that ψ_e is quadratic and $\psi_e'' = \beta_\psi$. Now, we use Lemma 10.6 to get the second assertion in (10.70):

$$
\begin{aligned}
&\left|\mathcal{E}_{\psi_e}(e_h^n) + \int_{\Omega_h^n} \psi_e'(e_h^n) e_h^n dS\right| \\
\lesssim& h^q \|y^n \circ \boldsymbol{\Phi}\|_{L^2(\Omega_h^n)} \|e_h^n\|_{L^2(\Omega_h^n)} + \beta_\psi h^{q+1} \|\nabla y^n\|_{L^2(\Omega_h^n)} \|e_h^n\|_{L^2(\Omega_h^n)} + \|e^n\|_{L^2(\Omega_h^n)} \|e_h^n\|_{L^2(\Omega_h^n)} \\
\lesssim& h^q \|y^n\|_{H^1(\Omega_h^n)} \|e_h^n\|_{L^2(\Omega_h^n)} + h^{m+1} \|y^n\|_{H^{m+1}(\Omega_h^n)} \|e_h^n\|_{L^2(\Omega_h^n)} \\
\lesssim& \left[h^q + h^{m+1}\right] \|y^n\|_{H^{m+1}(\Omega_h^n)} \|e_h^n\|_{L^2(\Omega_h^n)}.
\end{aligned}
$$

□

Lemma 10.12. *Assume $y^n \in H^{m+1}(\Omega)$ for $m \geq 1$. Then, we have the following estimates:*

$$\begin{aligned}
|\mathcal{E}_{\phi_c}(z_h)| &:= \left| \int_{\Gamma_h^n} \phi_c'(y_h^n) z_h dS - \int_{\Gamma^n} \phi_c'(y^n) z_h^\ell dS \right| \\
&\lesssim [h^q + h^m] \, \|y^n\|_{H^{m+1}(\Omega_h^n)} \|z_h\|_{H^1(\Omega_h^n)} + \|e_h^n\|_{H^1(\Omega_h^n)} \, \|z_h\|_{L^2(\Gamma_h^n)}, \\
\left| \mathcal{E}_{\phi_e}(e_h^n) + \int_{\Gamma_h^n} \phi_e'(e_h^n) e_h^n dS \right| &:= \left| \int_{\Gamma_h^n} \phi_e'(y_h^n) z_h dS - \int_{\Gamma^n} \phi_e'(y^n) z_h^\ell dS + \int_{\Gamma_h^n} \phi_e'(e_h^n) e_h^n dS \right| \\
&\lesssim [h^q + h^m] \, \|y^n\|_{H^{m+1}(\Omega_h^n)} \|e_h^n\|_{H^1(\Omega_h^n)}.
\end{aligned} \tag{10.75}$$

This results in the following estimate:

$$\begin{aligned}
&\left| \mathcal{E}_{\phi}(e_h^n) + \int_{\Gamma_h^n} \phi_e'(e_h^n) e_h^n dS \right| \\
&\qquad \lesssim [h^q + h^m] \, \|y^n\|_{H^{m+1}(\Omega_h^n)} \|e_h^n\|_{H^1(\Omega_h^n)} + \|e_h^n\|_{H^1(\Omega_h^n)} \, \|e_h^n\|_{L^2(\Gamma_h^n)}.
\end{aligned} \tag{10.76}$$

Proof. Using a change of variables, we have the following:

$$\int_{\Gamma^n} \phi_c'(y^n) z_h^\ell dS = \int_{\Gamma_h^n} \phi_c'(y^n \circ \mathbf{\Phi}) z_h \mu_h dS.$$

Now using the fundamental theorem of calculus for line integrals and some standard techniques we get

$$\begin{aligned}
&|\mathcal{E}_{\phi_c}(z_h)| \\
=& \left| \int_{\Gamma_h^n} \phi_c'(y_h^n) z_h dS - \int_{\Gamma^n} \phi_c'(y^n) z_h^\ell dS \right| \\
=& \left| \int_{\Gamma_h^n} \phi_c'(y_h^n) z_h dS - \int_{\Gamma_h^n} \phi_c'(y^n \circ \mathbf{\Phi}) z_h \mu_h dS \right| \\
\leq& \left| \int_{\Gamma_h^n} \phi_c'(y^n \circ \mathbf{\Phi}) z_h \left[\mu_h - 1\right] dS \right| + \left| \int_{\Gamma_h^n} \left[\phi_c'(y_h^n) - \phi_c'(y^n \circ \mathbf{\Phi})\right] z_h dS \right| \\
\lesssim& h^q \int_{\Gamma_h^n} |\phi_c'(y^n \circ \mathbf{\Phi}) z_h| \, dS + \left| \int_{\Gamma_h^n} \left[\phi_c'(y^n) - \phi_c'(y^n \circ \mathbf{\Phi})\right] z_h dS \right| + \left| \int_{\Gamma_h^n} \left[\phi_c'(y_h^n) - \phi_c'(y^n)\right] z_h dS \right| \\
\lesssim& h^q \int_{\Gamma_h^n} |\phi_c'(y^n \circ \mathbf{\Phi}) z_h| \, dS + \left| \int_{\Gamma_h^n} (y^n - y^n \circ \mathbf{\Phi}) z_h dS \right| + \left| \int_{\Gamma_h^n} (y_h^n - y^n) z_h dS \right|,
\end{aligned} \tag{10.77}$$

where we have used the geometry approximation and the fact that ϕ has quadratic growth and satisfies (9.11). Next, we use Hölder's inequality on all three terms. Due to a trace theorem we have that $z_h \in H^1(\Omega_h^n) \implies z_h \in L^4(\Gamma_h^n)$ for $\Omega_h^n \subset \mathbb{R}^3$. So,

$$
\begin{aligned}
&|\mathcal{E}_{\phi_c}(z_h)| \\
\lesssim & h^q \|\phi_c'(y^n \circ \mathbf{\Phi})\|_{L^2(\Gamma_h^n)} \|z_h\|_{L^2(\Gamma_h^n)} \\
&\qquad + h^{q+1} \|\nabla y^n\|_{L^2(\Gamma_h^n)} \|z_h\|_{L^2(\Gamma_h^n)} + \|y_h^n - y^n\|_{L^2(\Gamma_h^n)} \|z_h\|_{L^2(\Gamma_h^n)} \\
\lesssim & h^q \|y^n \circ \mathbf{\Phi}\|_{L^2(\Gamma_h^n)} \|z_h\|_{L^2(\Gamma_h^n)} \\
&\qquad + h^{q+1} \|\nabla y^n\|_{L^2(\Gamma_h^n)} \|z_h\|_{L^2(\Gamma_h^n)} + \|\mathbb{E}^n\|_{L^2(\Gamma_h^n)} \|z_h\|_{L^2(\Gamma_h^n)} \qquad (10.78) \\
\lesssim & h^q \|y^n\|_{H^1(\Omega_h^n)} \|z_h\|_{H^1(\Omega_h^n)} \\
&\qquad + h^{q+1} \|y^n\|_{H^2(\Omega_h^n)} \|z_h\|_{H^1(\Omega_h^n)} + \left[\|e_h^n\|_{H^1(\Omega_h^n)} + \|e^n\|_{H^1(\Omega_h^n)}\right] \|z_h\|_{L^2(\Gamma_h^n)} \\
\lesssim & h^q \|y^n\|_{H^2(\Omega_h^n)} \|z_h\|_{H^1(\Omega_h^n)} + h^m \|y^n\|_{H^{m+1}(\Omega_h^n)} \|z_h\|_{H^1(\Omega_h^n)} + \|e_h^n\|_{H^1(\Omega_h^n)} \|z_h\|_{L^2(\Gamma_h^n)} \\
\lesssim & \left[h^q + h^m\right] \|y^n\|_{H^{m+1}(\Omega_h^n)} \|z_h\|_{H^1(\Omega_h^n)} + \|e_h^n\|_{H^1(\Omega_h^n)} \|z_h\|_{L^2(\Gamma_h^n)},
\end{aligned}
$$

where we have used Lemma 10.6, the fact that ϕ has quadratic growth, the geometry approximation between Ω^n and Ω_h^n, and Corollary 4.13. For the other inequality, we have

$$\begin{aligned}
&\left|\mathcal{E}_{\phi_e}(e_h^n) + \int_{\Gamma_h^n} \phi_e'(e_h^n) e_h^n dS\right| \\
=&\left|\int_{\Gamma_h^n} \phi_e'(y_h^n) e_h^n dS - \int_{\Gamma^n} \phi_e'(y^n)(e_h^n)^\ell dS + \int_{\Gamma_h^n} \phi_e'(e_h^n) e_h^n dS\right| \\
=&\left|\int_{\Gamma_h^n} \phi_e'(y_h^n) e_h^n - \phi_e'(y^n \circ \mathbf{\Phi}) e_h^n \mu_h dS + \int_{\Gamma_h^n} \phi_e'(e_h^n) e_h^n dS\right| \\
\leq&\left|\int_{\Gamma_h^n} \phi_e'(y^n \circ \mathbf{\Phi}) e_h^n \left[\mu_h - 1\right] dS\right| + \left|\int_{\Gamma_h^n} \left[\phi_e'(y_h^n) - \phi_e'(y^n \circ \mathbf{\Phi}) + \phi_e'(e_h^n)\right] e_h^n dS\right| \\
\lesssim& h^q \int_{\Gamma_h^n} \left|\phi_e'(y^n \circ \mathbf{\Phi}) e_h^n\right| dS + \left|\int_{\Gamma_h^n} \left[\phi_e'(y_I^n) - \phi_e'(y^n \circ \mathbf{\Phi})\right] e_h^n dS\right| \\
\lesssim& h^q \int_{\Gamma_h^n} \left|\phi_e'(y^n \circ \mathbf{\Phi}) e_h^n\right| dS + \left|\int_{\Gamma_h^n} \left[\phi_e'(y^n) - \phi_e'(y^n \circ \mathbf{\Phi})\right] e_h^n dS\right| + \left|\int_{\Gamma_h^n} \left[\phi_e'(y_I^n) - \phi_e'(y^n)\right] e_h^n dS\right| \\
\lesssim& h^q \int_{\Gamma_h^n} \left|\phi_e'(y^n \circ \mathbf{\Phi}) e_h^n\right| dS + \left|\int_{\Gamma_h^n} \beta_\phi (y^n - y^n \circ \mathbf{\Phi}) e_h^n dS\right| + \left|\int_{\Gamma_h^n} \phi_e'(e^n) e_h^n dS\right|,
\end{aligned} \tag{10.79}$$

where we have used the fact that ϕ_e is quadratic and $\phi_e'' = \beta_\phi$. Now, we use (9.11) and Lemma 10.6 to get the second assertion in (10.75):

$$\begin{aligned}
&\left|\mathcal{E}_{\phi_e}(e_h^n) + \int_{\Gamma_h^n} \phi_e'(e_h^n) e_h^n dS\right| \\
\lesssim& h^q \|y^n \circ \mathbf{\Phi}\|_{L^2(\Gamma_h^n)} \|e_h^n\|_{L^2(\Gamma_h^n)} + \beta_\phi h^{q+1} \|\nabla y^n\|_{L^2(\Gamma_h^n)} \|e_h^n\|_{L^2(\Gamma_h^n)} + \|e^n\|_{L^2(\Gamma_h^n)} \|e_h^n\|_{L^2(\Gamma_h^n)} \\
\lesssim& h^q \|y^n\|_{H^2(\Omega_h^n)} \|e_h^n\|_{L^2(\Gamma_h^n)} + h^m \|y^n\|_{H^{m+1}(\Omega_h^n)} \|e_h^n\|_{L^2(\Gamma_h^n)} \\
\lesssim& \left[h^q + h^m\right] \|y^n\|_{H^{m+1}(\Omega_h^n)} \|e_h^n\|_{H^1(\Omega_h^n)},
\end{aligned}$$

□

The goal is to prove the following consistency estimate using similar techniques as Theorem 10.5. One needs to deal with the nonlinearities using convex splitting in order to obtain this estimate.

Theorem 10.13 (Consistency Estimate)**.** *Assume* $y^n \in W^{2,\infty}(\mathcal{C}) \cap L^\infty([0,T]; H^{m+1}(\Omega(t)))$

and $\partial_t y^n \in L^\infty([0,T]; H^m(\Omega(t)))$. Then, we have the following:

$$\begin{aligned}\|\mathbb{E}^k\|^2_{L^2(\Omega_h^k)} + \frac{\alpha}{4}\delta t \sum_{n=1}^{k}\left[\|\nabla \mathbb{E}^n\|^2_{L^2(\Omega_h^n)} + \gamma_{\mathrm{s}} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; \mathbb{E}^n, \mathbb{E}^n)\right] \\ \lesssim \exp\left(\left(C_2 + \zeta_h'' + \frac{C_4}{2}\right) t_k\right) R(y)\left(\delta t^2 + h^{2q} + h^{2m} K\right),\end{aligned} \tag{10.80}$$

where C_1 and C_2 are constants that depend on the estimates of the extension operator, and

$$R(y) = \sup_{t\in[0,T]}\left[\|y\|^6_{H^{m+1}(\Omega(t))} + \|y_t\|^2_{H^m(\Omega(t))} + C\right] + \|y\|^2_{W^{2,\infty}(\mathbb{Q})}.$$

Proof. Recall (10.53) and test with $z_h = 2\delta t e_h^n$

$$\begin{aligned}2\int_{\Omega_h^n}(e_h^n - e_h^{n-1})e_h^n d\boldsymbol{x} + 2\delta t a_h^n(e_h^n, e_h^n) + 2\gamma_{\mathrm{s}}\delta t s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; e_h^n, e_h^n) \\ = \mathcal{E}_I(2\delta t e_h^n) + \mathcal{E}_0(2\delta t e_h^n) + \mathcal{E}_\psi(2\delta t e_h^n) + \mathcal{E}_\phi(2\delta t e_h^n),\end{aligned} \tag{10.81}$$

and note that we have the following relation:

$$\begin{aligned}2\int_{\Omega_h^n}(e_h^n - e_h^{n-1})e_h^n d\boldsymbol{x} &= \int_{\Omega_h^n} 2(e_h^n)^2 - 2e_h^n e_h^{n-1} + (e_h^{n-1})^2 - (e_h^{n-1})^2 d\boldsymbol{x} \\ &= \|e_h^n\|^2_{L^2(\Omega_h^n)} - \|e_h^{n-1}\|^2_{L^2(\Omega_h^n)} + \|e_h^n - e_h^{n-1}\|^2_{L^2(\Omega_h^n)} \\ &\geq \|e_h^n\|^2_{L^2(\Omega_h^n)} - \|e_h^{n-1}\|^2_{L^2(\Omega_h^n)}.\end{aligned}$$

We also use a lower bound on $a_h^n(\cdot,\cdot)$ (which follows from Lemma 10.4):

$$a_h^n(e_h^n, e_h^n) + \int_{\Omega_h^n}\psi_e'(e_h^n)e_h^n d\boldsymbol{x} + \int_{\Gamma_h^n}\phi_e'(e_h^n)e_h^n dS \geq \frac{\alpha}{2}\|\nabla e_h^n\|^2_{L^2(\Omega_h^n)} - \zeta_h'\|e_h^n\|^2_{L^2(\Omega_h^n)}.$$

Then, we get the following:

$$(1 - 2\zeta_h'\delta t)\|e_h^n\|^2_{L^2(\Omega_h^n)} + \alpha\delta t\|\nabla e_h^n\|^2_{L^2(\Omega_h^n)} + 2\gamma_{\mathrm{s}}\delta t s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; e_h^n, e_h^n) \leq \mathcal{E}^n + \|e_h^{n-1}\|^2_{L^2(\Omega_h^n)}, \tag{10.82}$$

where $\mathcal{E}^n = 2\delta t\left[\mathcal{E}_I(e_h^n) + \mathcal{E}_0(e_h^n) + \mathcal{E}_\psi(e_h^n) + \int_{\Omega_h^n}\psi_e'(e_h^n)e_h^n d\boldsymbol{x} + \mathcal{E}_\phi(e_h^n) + \int_{\Gamma_h^n}\phi_e'(e_h^n)e_h^n dS\right]$ contains the error terms. Next, using Lemmas 5.5 and 5.7 from [50], we get the following estimates for $\|e_h^{n-1}\|^2_{L^2(\Omega_h^n)}$ that hold for all $0 \le n \le N$ for constants C_1, C_2, C_3 that do not depend on n:

$$\|e_h^0\|^2_{L^2(\Omega_h^1)} \le \|e_h^0\|^2_{L^2(\mathcal{O}_\delta(\Omega_h^0)} \le C_1\|e_h^0\|^2_{L^2(\Omega_h^0)} + C_1 K h^2 s_h(\mathcal{F}^0_{\Sigma_\delta^\pm}; e_h^0, e_h^0),$$

$$\begin{aligned}\|e_h^{n-1}\|^2_{L^2(\Omega_h^n)} &\le \|e_h^{n-1}\|^2_{L^2(\mathcal{O}_\delta(\Omega_h^{n-1})}\\ &\le (1 + C_2\delta t)\|e_h^{n-1}\|^2_{L^2(\Omega_h^{n-1})} + \frac{\alpha}{2}\delta t\|\nabla e_h^{n-1}\|^2_{L^2(\Omega_h^{n-1})} + C_3\delta t K s_h(\mathcal{F}^{n-1}_{\Sigma_\delta^\pm}; e_h^{n-1}, e_h^{n-1}).\end{aligned} \tag{10.83}$$

Now, by summing up (10.82) over $n = 1, ..., k$, we get the following:

$$\begin{aligned}(1 - 2\delta t\zeta_h')\sum_{n=1}^{k}\|e_h^n\|^2_{L^2(\Omega_h^n)} + \alpha\delta t\sum_{n=1}^{k}\|\nabla e_h^n\|^2_{L^2(\Omega_h^n)} + 2\delta t\gamma_{\mathrm{s}}\sum_{n=1}^{k} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; e_h^n, e_h^n)\\ \le \sum_{n=1}^{k}\mathcal{E}^n + \sum_{n=1}^{k}\|e_h^{n-1}\|^2_{L^2(\Omega_h^n)}.\end{aligned} \tag{10.84}$$

Then, by applying (10.83) and choosing $\gamma_s \ge C_3 K$, we get

$$\begin{aligned}(1 - 2\delta t\zeta_h')\|e_h^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{2}\delta t\sum_{n=1}^{k}\|\nabla e_h^n\|^2_{L^2(\Omega_h^n)} + \delta t\gamma_{\mathrm{s}}\sum_{n=1}^{k} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; e_h^n, e_h^n)\\ \le \sum_{n=1}^{k}\mathcal{E}^n + C_1\|e_h^0\|^2_{L^2(\Omega_h{}^0)} + C_1 K h^2 s_h(\mathcal{F}^0_{\Sigma_\delta^\pm}; e_h^0, e_h^0) + \delta t\sum_{n=2}^{k}(C_2 + 2\zeta_h')\|e_h^{n-1}\|^2_{L^2(\Omega_h^{n-1})}.\end{aligned} \tag{10.85}$$

Now, by using the two estimates of the double well potentials from Lemmas 10.11 and 10.12 and Lemmas 10.9 and 10.10 with a weighted Young's inequality, we have the following estimate of $\sum\limits_{n=1}^{k}\mathcal{E}^n$:

$$\sum_{n=1}^{k}\mathcal{E}^n \le C\delta t\left[\delta t^2 + h^{2q} + h^{2m}K\right]R(y) + \frac{\delta t}{2}\sum_{n=1}^{k}\left[C_4\|e_h^n\|^2_{L^2(\Omega_h^n)} + \frac{\alpha}{2}\|\nabla e_h^n\|^2_{L^2(\Omega_h^n)} + \gamma_{\mathrm{s}} s_h(e_h^n, e_h^n)\right], \tag{10.86}$$

where C_4 is independent of h and δt and depends on the weighting of the Young's inequalities and $R(y) = \sup_{t\in[0,T]}\left[\|y\|^6_{H^{m+1}(\Omega(t))} + \|y_t\|^2_{H^m(\Omega(t))} + C\right] + \|y\|^2_{W^{2,\infty}(\mathbb{Q})}$. Then, by choosing $\delta t \zeta_h' < \frac{1}{4}$, substituting (10.86), and noting that $e_h^0 = 0$ on $\mathcal{O}_\delta(\Omega_h^n)$, we have

$$\begin{aligned} &\|e_h^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{2}\delta t \sum_{n=1}^{k} \|\nabla e_h^n\|^2_{L^2(\Omega_h^n)} + \delta t \gamma_{\mathrm{s}} \sum_{n=1}^{k} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; e_h^n, e_h^n) \\ &\quad \le C\delta t \left[\delta t^2 + h^{2q} + h^{2m}\right] R(y) + \delta t \sum_{n=2}^{k} \left(C_2 + 2\zeta_h' + \frac{C_4}{2}\right) \|e_h^{n-1}\|^2_{L^2(\Omega_h^{n-1})}. \end{aligned} \tag{10.87}$$

Now, by the discrete Gronwall inequality stated in Lemma 1 of the appendix, we get the following:

$$\begin{aligned} &\|e_h^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{2}\delta t \sum_{n=1}^{k} \|\nabla e_h^n\|^2_{L^2(\Omega_h^n)} + \delta t \gamma_{\mathrm{s}} \sum_{n=1}^{k} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; e_h^n, e_h^n) \\ &\quad \lesssim \exp\left(\left(C_2 + \zeta_h'' + \frac{C_4}{2}\right) t_k\right) R(y) \left(\delta t^2 + h^{2q} + h^{2m} K\right). \end{aligned} \tag{10.88}$$

Then, by using a triangle inequality with a standard interpolation result we get

$$\begin{aligned} &\|\mathbb{E}^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{2}\delta t \sum_{n=1}^{k} \|\nabla \mathbb{E}^n\|^2_{L^2(\Omega_h^n)} + \delta t \gamma_{\mathrm{s}} \sum_{n=1}^{k} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; \mathbb{E}^n, \mathbb{E}^n) \\ &\quad \lesssim \exp\left(\left(C_2 + \zeta_h'' + \frac{C_4}{2}\right) t_k\right) R(y) \left(\delta t^2 + h^{2q} + h^{2m} K\right) \\ &\qquad + \|e^k\|^2_{L^2(\Omega^k)} + \frac{\alpha}{2}\delta t \sum_{n=1}^{k} \|\nabla e^n\|^2_{L^2(\Omega_h^n)} + \delta t \gamma_{\mathrm{s}} \sum_{n=1}^{k} s_h(\mathcal{F}^n_{\Sigma_\delta^\pm}; e^n, e^n) \\ &\quad \lesssim \exp\left(\left(C_2 + \zeta_h'' + \frac{C_4}{2}\right) t_k\right) R(y) \left(\delta t^2 + h^{2q} + h^{2m} K\right) + \sup_{t\in[0,T]} \|y\|^2_{H^{m+1}(\Omega(t))} h^{2m} K \\ &\quad \lesssim \exp\left(\left(C_2 + \zeta_h'' + \frac{C_4}{2}\right) t_k\right) R(y) \left(\delta t^2 + h^{2q} + h^{2m} K\right). \end{aligned} \tag{10.89}$$

□

Hence, with this theorem, the unfitted finite element scheme is consistent for the Allen–Cahn problem with the nonlinear double well potentials.

Chapter 11. Remarks on an Unfitted Method for Allen–Cahn

In Chapter 9, we provided a brief overview of the Landau–de Gennes model along with some basic theory. We also introduced the Beris–Edwards system for the Landau–de Gennes model so that we can consider time-dependent domains. Our current work assumes a prescribed motion of the domain, but we aim to relax this assumption in future research.

Lastly, in Chapter 10, we established a consistency estimate for a modified Allen–Cahn equation which can be extended to the Landau–de Gennes model. The analysis for the Landau–de Gennes model with an unfitted framework should follow very similarly since they share the same type of nonlinearities (i.e. they both have double well potentials). Note that some additional terms need to be accounted for when incorporating the (half) Beris–Edwards system, namely the term $B\left(\nabla \mathbf{v}, Q\right)$ in (9.27). But this can be easily dealt with under the assumption of a prescribed motion of the domain, i.e for a given $\mathbf{v}$.

Appendix

The following lemma from [72] is needed in the analysis of the Allen–Cahn problem in Chapter 10

Lemma 1. *(Discrete Grönwall Inequality) Let u_k satisfy*

$$u_n \leq \alpha_n + \sum_{k=0}^{n-1} \beta_k u_k, \quad \forall n \geq 0, \tag{1}$$

where α_n is nondecreasing and $\beta_n \geq 0$. Then it follows that

$$u_n \leq \alpha_n \exp\left(\sum_{k=0}^{n-1} \beta_k\right). \tag{2}$$

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Vita

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