OPTIMAL CONTROL OF A FREE BOUNDARY PROBLEM WITH SURFACE TENSION EFFECTS: A PRIORI ERROR ANALYSIS

HARBIR ANTIL†, RICARDO H. NOCHETTO‡, AND PATRICK SODRÉ§

Abstract. We present a finite element method along with its analysis for the optimal control of a model free boundary problem with surface tension effects, formulated and studied in [1]. The state system couples the Laplace equation in the bulk with the Young-Laplace equation on the free boundary to account for surface tension. We first prove that the state and adjoint system have the requisite regularity for the error analysis (strong solutions). We discretize the state, adjoint and control variables via piecewise linear finite elements and show optimal $O(h)$ error estimates for all variables, including the control. This entails using the second order sufficient optimality conditions of [1], and the first order necessary optimality conditions for both the continuous and discrete systems. We conclude with two numerical examples which examine the various error estimates.

Key words. sharp interface model, free boundary, curvature, surface tension, pde constrained optimization, boundary control, finite element method, L2 projection, second order sufficient conditions, a priori error estimate.

AMS subject classifications. 49J20, 35Q93, 35Q35, 35R35, 65N30.

1. Introduction. The purpose of this paper is to numerically analyze the optimal control problem we proposed in [1]. The underlying state system couples the Laplace equation in the bulk with the Young-Laplace equation on the free boundary to account for surface tension, as proposed by P. Saavedra and L. R. Scott in [11]. We first recall the continuous optimal control problem from [1, Section 2].

Fig. 1.1. $\Omega_\gamma$ denotes a physical domain with boundary $\partial\Omega_\gamma = \Sigma \cup \Gamma_\gamma$. Here $\Sigma$ includes the lateral and the bottom boundary and is assumed to be fixed. Furthermore, the top boundary $\Gamma_\gamma$ (dotted line) is “free” and is assumed to be a graph of the form $(x_1, 1 + \gamma(x_1))$, where $\gamma \in W^1_\infty(0, 1)$ denotes a parametrization. The free boundary $\Gamma_\gamma$ is further mapped to a fixed boundary $\Gamma = (0, 1) \times \{1\}$ and in turn the physical domain $\Omega_\gamma$ is mapped to a reference domain $\Omega = (0, 1)^2$, where all computations are carried out.

Let $\gamma \in W^1_\infty(0, 1)$ denote a parametrization of the top boundary (see Figure 1).

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†Department of Mathematical Sciences. George Mason University, Fairfax, VA 22030, USA (hantil@gmu.edu).
‡Department of Mathematics and Institute for Physical Science and Technology, University of Maryland College Park, MD 20742, USA (rhn@math.umd.edu).
§Department of Mathematics, University of Maryland College Park, MD 20742, USA (sodre@math.umd.edu).
of the physical domain \( \Omega \subset \Omega^* \subset \mathbb{R}^2 \) with boundary \( \partial \Omega := \Gamma \cup \Sigma \), defined as

\[ \begin{aligned} \Omega^* &:= (0, 1) \times (0, 2), \\
\Omega_\gamma &:= \{ (x_1, x_2) : 0 < x_1 < 1, 0 < x_2 < 1 + \gamma(x_1) \}, \\
\Gamma_\gamma &:= \{ (x_1, x_2) : 0 < x_1 < 1, x_2 = 1 + \gamma(x_1) \}, \\
\Sigma &:= \partial \Omega_\gamma \setminus \Gamma_\gamma, \\
\Gamma &:= \{ (x_1, x_2) : 0 < x_1 < 1, x_2 = 1 \}. \end{aligned} \]

Here, \( \Omega^* \) and \( \Sigma \) are fixed while \( \Omega_\gamma \) and \( \Gamma_\gamma \) deform according to \( \gamma \).

We want to find an optimal control \( u \in U_{ad} \subset L^2(0, 1) \) so that the solution pair \((\gamma, y)\) to the free boundary problem (FBP) is the best least squares fit of desired boundary \( \gamma_d : (0, 1) \to \mathbb{R} \) and bulk \( y_d : \Omega^* \to \mathbb{R} \) configurations. This amounts to solving the problem: minimize

\[
\mathcal{J}(\gamma, y, u) := \frac{1}{2} \| \gamma - \gamma_d \|^2_{L^2(0,1)} + \frac{1}{2} \| y - y_d \|^2_{L^2(\Omega_\gamma)} + \frac{\lambda}{2} \| u \|^2_{L^2(0,1)},
\]

subject to the state equations

\[
\begin{cases} 
- \Delta y = 0 & \text{in } \Omega_\gamma \\
y = v & \text{on } \partial \Omega_\gamma \\
- \kappa \mathcal{H}[\gamma] + \partial_{x_1} y (\cdot, 1 + \gamma) = u & \text{on } (0, 1)^2 \\
\gamma(0) = \gamma(1) = 0,
\end{cases}
\]

the state constraints

\[
|d_{x_1}\gamma| \leq 1 \quad \text{a.e. in } (0, 1),
\]

with \( d_{x_1} \) being the total derivative with respect to \( x_1 \), and the control constraint

\[
u \in U_{ad}
\]

dictated by \( U_{ad} \), a closed ball in \( L^2(0, 1) \), to be specified later in (2.6). Here \( \lambda > 0 \) is the stabilization parameter; \( v \) is given data which in principle could act as a Dirichlet boundary control:

\[
\mathcal{H}[\gamma] := d_{x_1} \left( \frac{d_{x_1}\gamma}{\sqrt{1 + |d_{x_1}\gamma|^2}} \right)
\]

is the curvature of \( \gamma \); and \( \kappa > 0 \) plays the role of surface tension coefficient.

We use a fixed domain approach to solve the optimal control free boundary problem (OC-FBP). In fact, we transform \( \Omega_\gamma \) to \( \Omega = (0, 1)^2 \) and \( \Gamma_\gamma \) to \( \Gamma = (0, 1) \times \{ 1 \} \) (see Figure [1]), at the expense of having a governing PDE with rough coefficients. One of the challenges of an OC-FBP is dealing with state constraints which may allow or prevent topological changes of the domain. Our analysis in [1] yields the control constraint (1.2d), which always enforce the state constraint (1.2c) i.e., we can treat OC-FBP as a simpler control constrained problem. Moreover, we proved novel second order sufficient conditions for the optimal control problem for small data \( v \). As a consequence we obtained that the above minimization has a (locally) unique solution.
In this paper we introduce the fully discrete optimization problem, using piecewise linear finite elements, and show that it converges with an optimal rate $O(h)$ for all variables. In fact, the convergence analysis for the control requires a-priori error estimates for both the state and the adjoint equations. The state equations error estimates were developed by P. Saavedra and R. Scott in [11] under the assumption that the continuous state equations have suitable second order regularity (strong Sobolev solutions). Our first goal is to prove such a regularity for $v \in W^p_2(\Omega), p > 2$, via a fixed-point argument, as well as to extend the analysis to the continuous adjoint equations. Our analysis of strong solutions for both the state and adjoint equations is novel in Sobolev spaces but not in Hölder spaces [12]. We exploit this second order regularity to derive a-priori error estimates for the state and adjoint variables based on [11]: the former are a direct extension of [11] whereas the latter are new. An important difference with [11] is the presence of the control variable $u$, for which we obtain also a novel a-priori error estimate.

There are two approaches for dealing with a discrete optimal control problem with PDE constraints. Both rely on an agnostic discretization of the state and adjoint equations, perhaps by the finite element method; they differ on whether or not the admissible set of controls is discretized as well. The first approach [2, 5, 10] follows a more physically appealing idea and also discretizes the admissible control set. The second approach [8] induces a discretization of the optimal control by projecting the discrete adjoint state into the admissible control set. From an implementation perspective this projection may lead to a control which is not discrete in the current mesh and thus requires an independent mesh. Its key advantage is obtaining an optimal quadratic rate of convergence [8, Theorem 2.4] for the control. We point that no such improvements can be inferred for our problem. This is due to the highly nonlinear nature of the state equations and the necessity to discretize the (rough) coefficients. We will provide more details on this topic in Section 6 below.

We follow the first approach and discretize the entire optimization problem using piecewise linear finite elements. However, we exploit the structure of the admissible control set and show optimal convergence rates for the state, adjoint, and control variables. We largely base our error analysis of the state and adjoint equations on the work by P. Saavedra and L. R. Scott [11]. For analyzing the discrete control we use the second order sufficient condition we developed in [1, Theorem 5.6] together with the first order necessary conditions for the continuous and discrete systems.

To prove well-posedness of the discrete state and adjoint systems we rely on the inf-sup theory and a fixed point argument. Therefore, the smallness assumption on the data $v$ is still required as in the continuous case [1, Theorem 4.5]. However, with the aid of simulations we are able to explore the control problem beyond theory and test it for large data.

The outline of this paper is as follows: In Section 2.1 we state the variational form for the OC-FBP. We summarize the first order necessary and second order sufficient conditions in Sections 2.2 and 2.3. For boundary data in $W^p_2, p > 2$, we show that the state and the adjoint systems have strong solutions in Section 3. We introduce a finite element discretization of the system in Section 4 and prove error estimates in $W^1_p \times W^1_\infty$ for the state variables and in $W^1_q \times W^1_1$ for the adjoint variables. We derive an $L^2$-error estimate for the optimal control in Section 6. We conclude with two numerical examples in Section 7 which confirm our theoretical findings: the first example explores the unconstrained problem, whereas the second example deals with the constrained one.
2. Continuous Optimal Control Problem. The purpose of this section is to recall the continuous optimal control problem in its variational form along with its first and second optimality conditions derived in [1]. We denote by \( \lesssim \) the inequality \( \leq C \) with a constant independent of the quantities of interest.

2.1. Problem Formulation. We choose to present the formulation directly in its variational form on the reference domain \( \Omega \) after having linearized the curvature \( \mathcal{H} \), and scaled the control \( u \). These assumptions, not being crucial [1] Section 2, \( A_1 - A_2 \), result in an optimal control problem subject to a nonlinear PDE constraint with (rough) coefficients depending on \( \gamma \) but without an explicit interface. We denote by \( B_\mathcal{H}: W_\infty^1 (0,1) \times W_1^1 (0,1) \rightarrow \mathbb{R} \) and \( B_\Omega : W_\infty^2 (\Omega) \times W_1^2 (\Omega) \rightarrow \mathbb{R} \) the bilinear forms

\[
B_\mathcal{H} \left[ \gamma, \xi \right] := \kappa \int_0^1 d_{x_1} \gamma(x_1) d_{x_1} \xi(x_1) \, dx_1,
\]

\[
B_\Omega \left[ y, z; A \left[ \gamma \right] \right] := \int_\Omega A \left[ \gamma \right] \nabla y \cdot \nabla z \, dx,
\]

with surface tension constant \( \kappa \). The coefficient matrix \( A \left[ \gamma \right] \) arises from mapping the physical domain \( \Omega \), to the reference domain \( \Omega \) and is given by [1] Section 2

\[
A \left[ \gamma \right] = \begin{bmatrix}
1 + \gamma(x_1) & -d_{x_1} \gamma(x_1)x_2 \\
-d_{x_1} \gamma(x_1)x_2 & 1 + \frac{(d_{x_1} \gamma(x_1)x_2)^2}{1 + \gamma(x_1)}
\end{bmatrix}.
\]

Let \( E : \tilde{W}_1^1 (0,1) \rightarrow W_\infty^1 (\Omega), 1 < q < 2 \), be a continuous linear extension operator, namely,

\[
E \xi |_R = \xi, \quad E \xi |_\Omega = 0, \quad |E \xi|_{W_q^1(\Omega)} \leq C_E |\xi|_{W_1^1(0,1)},
\]

where \( C_E \) is the stability constant. It is convenient to introduce the product space:

\[
W_{t,s}^1 := \tilde{W}_t^1 (0,1) \times \tilde{W}_s^1 (\Omega) \quad 1 \leq t, s \leq \infty.
\]

Given \( v \in W_\infty^1 (\Omega) \), a lifting of the boundary data to \( \Omega \), \( y_d \in L^2(\Omega^*), \gamma_d \in L^2(0,1) \), let \( \delta y := y + v - y_d \), \( \delta \gamma := \gamma - \gamma_d \). The optimal control problem is to minimize

\[
J \left( \gamma, y, u \right) := \frac{1}{2} \| \delta \gamma \|_{L^2(0,1)}^2 + \frac{1}{2} \| \delta y \sqrt{1 + \gamma} \|_{L^2(\Omega)}^2 + \frac{\lambda}{2} \| u \|_{L^2(0,1)}^2,
\]

with state variable \( \left( \gamma, y \right) \in W_{t,s}^1 \), \( p > 2 \) satisfying the state equations

\[
B_\mathcal{H} \left[ \gamma, \xi \right] + B_\Omega \left[ y + v, z + E \xi; A \left[ \gamma \right] \right] = \langle u, \xi \rangle_{W_{-1}^\infty(0,1) \times \tilde{W}_1^1(0,1)} \quad \forall \left( \xi, z \right) \in W_{t,s}^1,
\]

the state constraint

\[
\left| d_{x_1} \gamma(x_1) \right| \leq 1 \quad \text{a.e.} \quad x_1 \in (0,1),
\]

with \( d_{x_1} \) being the total derivative with respect to \( x_1 \), and the control constraint

\[
u \in \mathcal{U}_{ad}.
\]
The set $\mathcal{U}_{ad}$ of admissible controls is a closed ball in $L^2(0,1)$ defined as follows: if $\theta_1 \in (0,1)$ is chosen as in [1 Lemma 4.3], and $\alpha$ is the inf-sup constant for $B_T$ [1 Proposition 4.1], then

$$
\mathcal{U}_{ad} := \left\{ u \in L^2(0,1) : \|u\|_{L^2(0,1)} \leq \theta_1/2\alpha \right\}.
$$

We also need the open ball $\mathcal{U} := \left\{ u \in L^2(0,1) : \|u\|_{L^2(0,1)} < \theta_1/\alpha \right\}$, so that $\mathcal{U}_{ad} \subset \mathcal{U}$.

In view of the regularity of $u$ and $\xi$, the duality pairing $\langle u, \xi \rangle_{W^{-1}_p(0,1) \times W^1_0(0,1)}$ reduces to $\int_0^1 u \xi$. We refer to [1 Equations 4.5-4.6] for details. Since $\mathcal{U}_{ad}$ is not open, we need to define a proper set of admissible directions to compute derivatives with respect to $u$. Given $u \in \mathcal{U}_{ad}$, the convex cone $C(u)$ comprises all directions $h \in L^2(0,1)$ such that $u + th \in \mathcal{U}_{ad}$, $t > 0$, i.e.,

$$
C(u) := \left\{ h \in L^2(0,1) : u + th \in \mathcal{U}_{ad}, t > 0 \right\}.
$$

The proof of existence and local uniqueness of a minimizer of (2.5) involves multiple steps. The first step [1 Subsection 4.1.1] is to impose a smallness condition on the data $v$ and restrict the radius of the $L^2(0,1)$ ball $\mathcal{U}_{ad}$ to solve the nonlinear system (2.5b)-(2.5c). The second step [1 Subsection 4.1.2] is to improve the regularity of $\gamma$ from Lipschitz continuous to the fractional Sobolev space $W^{2-1/p}_p(0,1)$. This additional regularity is in turn used to prove the existence of a minimizer in [1 Subsection 5.1]. The last two steps [1 Subsection 5.2 and 5.3] consist of computing the first and second order optimality conditions.

The optimality conditions are essential tools for this paper. From the simulation perspective, the first order condition yields a way to compute a minimizing sequence. From a numerical analysis perspective, the second order condition is the starting point for proving an a-priori error estimate. We recall now these conditions and prove a new result, Lemma 2.1, which is instrumental for implementing the adjoint system.

### 2.2. First-order Optimality Condition

The purpose of this section is to state the first order necessary optimality conditions using the reduced cost functional approach; a formal Lagrange multiplier approach is also presented in [1 Section 3].

Given $u \in \mathcal{U}$, there exists a unique solution $(\gamma, y) \in W_{\infty, p}^{1,1}$ of (2.5b)-(2.5c). This induces the so-called control-to-state map $G_v : \mathcal{U} \rightarrow W_{\infty, p}^{1,1}$, where $G_v(u) = (\gamma(u), y(u))$, and we can write the cost functional $\mathcal{J}$ in (2.5a) in the reduced form as

$$
\mathcal{J}(u) := \mathcal{J}_1(G_v(u)) + \mathcal{J}_2(u)
$$

with

$$
\mathcal{J}_1(\gamma, y) := \frac{1}{2} \|\delta y\|_{L^2(0,1)}^2 + \frac{1}{2} \|\delta y \sqrt{1 + \gamma}\|_{L^2(\Omega)}^2, \quad \mathcal{J}_2(u) = \frac{\lambda}{2} \|u\|_{L^2(0,1)}^2.
$$

Therefore, if $\bar{u} \in \mathcal{U}_{ad}$ is a minimizer of $\mathcal{J}$, then $\bar{u}$ satisfies the variational inequality

$$
\langle \mathcal{J}'(\bar{u}), u - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} \geq 0 \quad \forall u \in \mathcal{U}_{ad}.
$$

Deriving an expression for $\mathcal{J}'(\bar{u})$ is one of the main difficulties of an optimization problem. It turns out that $\mathcal{J}'(\bar{u}) = \lambda \bar{u} + \bar{s}$ [1 Sections 3 and 5.2], whence

$$
\langle \lambda \bar{u} + \bar{s}, u - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} \geq 0 \quad \forall u \in \mathcal{U}_{ad},
$$
where \((\bar{s}, \bar{r} - E\bar{s}) \in W_{1,q}^1\) and \((\bar{s}, \bar{r})\) satisfies the adjoint equations in variational form
\[
B_T [\xi, \bar{s}] + D_\Omega [(\xi, z), \bar{r}; \bar{\gamma}, \bar{y}] = \langle f' (\bar{\gamma}, \bar{y}), (\xi, z) \rangle \\
= \langle \xi, \delta \bar{\gamma} + \frac{1}{2} \int_0^1 |\delta \bar{y}|^2 \, dx_2 \rangle + \langle z, \delta \bar{y} (1 + \bar{\gamma}) \rangle,
\]
(2.10)
for all \((\xi, z) \in W_{1,\infty,p}^1\) with \((\bar{\gamma}, \bar{y}) := (\gamma (\bar{u}), y (\bar{u}))\), where \(D_\Omega\) is the parametrized form
\[
D_\Omega [(\xi, z), \bar{r}; \bar{\gamma}, \bar{y}] := B_T [\xi, \bar{r}; A [\bar{\gamma}]] + B_\Omega [\bar{y} + v, \bar{r}; D A [\bar{\gamma}]; \xi]
\]
(2.11)
with derivative of \(A\) with respect to \(\gamma\) given by \(D A [\bar{\gamma}]; h) = A_1 [\bar{\gamma}] h + A_2 [\bar{\gamma}] d_\gamma h\) \((2.4)\). Moreover, the duality pairings on the right hand side of (2.10) are reduced to standard integrals due to the \(L^2\)-regularity imposed by the cost functional.

The assembly of (2.10) is nontrivial. In view of (2.1) and (2.11) we have
\[
B_\Omega [\bar{y} + v, \bar{r}; D A [\bar{\gamma}]; \xi] = \int_0^1 \left( \int_0^1 A_1 [\bar{\gamma}] \nabla (\bar{y} + v) \cdot \nabla \bar{r} \, dx_2 \right) \xi \, dx_1 \\
+ \int_0^1 \left( \int_0^1 A_2 [\bar{\gamma}] \nabla (\bar{y} + v) \cdot \nabla \bar{r} \, dx_2 \right) \xi, \, dx_1,
\]
(2.12)
and the computation of the inner integrals in the variable \(x_2\) alone might seem like a daunting task. However we can circumvent this issue altogether with the following simple observation. The control-to-state map \(G_v : U \to W_{\infty,\infty}^1\) admits a Fréchet derivative \((\gamma, y) = G'_v (\bar{u}) h \in W_{\infty,\infty}^1\) which satisfies the linear variational system
\[
B_T [\gamma, \zeta] + D_\Omega [(\gamma, y), z + E \zeta; \bar{\gamma}, \bar{y}] = \int_0^1 h \zeta \quad \forall (\zeta, z) \in W_{1,\infty,q}^1.
\]
(2.14)
for every \(\bar{u} \in U\) and \(h \in L^2(0, 1)\). This formal differentiation of (2.5b) is rigorously justified in [1, Theorem 4.12]. The system (2.14) consists of the two equations
\[
B_\Omega [y, z, A [\bar{\gamma}]] + B_\Omega [\bar{y} + v, z; D A [\bar{\gamma}]; \langle \gamma \rangle] = 0 \quad \forall z \in W_q^1 (\Omega) \\
B_\Omega [y, E \zeta; A [\bar{\gamma}]] + B_\Omega [\bar{y} + v, E \zeta; D A [\bar{\gamma}]; \langle \gamma \rangle] + B_T [\gamma, \zeta] = \langle h, \zeta \rangle \quad \forall \zeta \in W_q^1 (0, 1).
\]
The formal adjoint of this system, obtained upon regarding \((\gamma, y) \in W_{\infty,\infty}^1\) as test functions and \((\zeta, z) \in W_{1,\infty,q}^1\) as unknowns, reads as follows:
\[
B_\Omega [y, z, A [\bar{\gamma}]] + B_\Omega [y, E \zeta; A [\bar{\gamma}]] = \langle f, y \rangle \\
B_\Omega [y + v, z; D A [\bar{\gamma}]; \langle \gamma \rangle] + B_\Omega [\bar{y} + v, E \zeta; D A [\bar{\gamma}]; \langle \gamma \rangle] + B_T [\gamma, \zeta] = \langle g, \zeta \rangle.
\]
(2.15)

Lemma 2.1 (relation between (2.10) and (2.15)). The linear system (2.10) coincides with (2.15) provided \(f = \delta \bar{y} (1 + \bar{\gamma})\) and \(g = \delta \bar{\gamma} + \frac{1}{2} \int_0^1 |\delta \bar{y}|^2 \, dx_2\).

Proof. It suffices to check that \((\zeta, z + E \zeta)\) satisfies (2.10) and invoke the uniqueness of (2.10), the latter being a consequence of [1, Lemma 5.6]. □

Lemma 2.2 is instrumental for the implementation of this control problem. Later in Section 7 we choose Newton’s method instead of a fixed point iteration to solve the state equations, because it is locally a second order method. Secondly, computing a Newton direction \((\gamma, y)\) requires solving a linear system of type (2.14). By transposition, the same matrix can be used to solve for the adjoint variables thereby making the seemingly complicated coupling \(D_\Omega\) rather simple to deal with.
2.3. Second-order Sufficient Conditions. It is well known that the first order necessary optimality conditions are also sufficient for the well-posedness of a convex optimization problem with linear constraints. Unfortunately, we cannot assert the convexity of our problem due to the highly nonlinear nature of (2.5a)-(2.5b). A large portion of our previous work [1, Theorem 5.7] was devoted to proving a second-order sufficient condition. We restrict ourselves to merely restating that result.

**Theorem 2.2 (second-order sufficient conditions).** If \( |v|_{W_1^p(\Omega)} \) is small enough and \( \bar{u} \) in \( U_{ad} \) is an optimal control, then there exists a neighborhood of \( \bar{u} \) such that

\[
J''(\bar{u})(u - \bar{u})^2 \geq \frac{\lambda}{2} ||u - \bar{u}||_{L^2(0,1)}^2 \quad \forall u \in \bar{u} + C(\bar{u}).
\]

(2.16)

Furthermore, the following two conditions hold: local quadratic growth

\[
J(u) = J(\bar{u}) + \frac{\lambda}{8} ||u - \bar{u}||_{L^2(0,1)}^2 \quad \forall u \in \bar{u} + C(\bar{u}),
\]

(2.17)

and local convexity

\[
\langle J'(u) - J'(\bar{u}), u - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} \geq \frac{\lambda}{4} ||u - \bar{u}||_{L^2(0,1)}^2 \quad \forall u \in \bar{u} + C(\bar{u}).
\]

(2.18)

3. Strong Solutions: Second-order Regularity. The goal of this section is to prove the existence of strong solutions to the state and adjoint equations. The underlying second-order Sobolev regularity is crucial for the a-priori error estimates of Section 5, and thus an important contribution of this paper.

3.1. Second-order Regularity in the Square. We start with an auxiliary regularity result for the square \( \Omega \). This type of results are well known for \( C^{1,1} \) domains [7, Theorem 9.15 and Lemma 9.17].

**Lemma 3.1 (second-order regularity in the square).** Let \( \Omega = (0,1)^2 \) and \( A = (a_{ij})_{i,j=1}^2 \in W_1^\infty(\Omega) \). If \( f \in L^p(\Omega) \), with \( 1 < p < \infty \), then there exists a unique solution \( w \in W_p^2(\Omega) \cap W_1^1(\Omega) \) to

\[
- \text{div}(A\nabla w) = f \quad \text{in} \; \Omega,
\]

(3.1)

and a constant \( C_\# \) depending on \( ||A||_{W_1^\infty(\Omega)} \) and \( p \) such that

\[
||w||_{W_p^2(\Omega)} \leq C_\# ||f||_{L^p(\Omega)}.
\]

(3.2)

**Proof.** We proceed in several steps. First we prove (3.2) assuming that there is a solution in \( W_2^p(\Omega) \), and next we show the existence of such a solution.

1. **Reflection.** We introduce an odd reflection \( \bar{f} \) of \( f \) and an even reflection \( \bar{A} \) of \( A \) to the adjacent unit squares of \( \Omega \) so that the extended domain \( \bar{\Omega} \) is a square with vertices \((-1, -1), (2, -1), (2, 2), (-1, 2)\). We observe that \( \bar{f} \in L^p(\bar{\Omega}) \) and \( \bar{A} \in W_1^\infty(\bar{\Omega}) \).

Since \( ||\bar{f}||_{H^{-1}(\bar{\Omega})} \lesssim ||\bar{f}||_{L^p(\bar{\Omega})} \) by Sobolev embedding in two dimensions, there exists a unique solution \( \bar{w} \in H_1^0(\bar{\Omega}) \) to the extended problem

\[
- \text{div}(\bar{A}\nabla \bar{w}) = \bar{f} \quad \text{in} \; \bar{\Omega}.
\]

(3.3)
domain for the fixed point iterator, linearizing the free boundary problem by freezing and \[1, Section 4.1.1\]. It consists of three steps: defining a convex set which acts as

$$\tilde{w}$$ is an odd reflection to \(\tilde{\Omega}\) of its restriction \(w\) to \(\Omega\), whence \(w\) has a vanishing trace on \(\partial\Omega\). Moreover, \(\|\tilde{w}\|_{L^p(\tilde{\Omega})} \lesssim \|\tilde{w}\|_{H^1_0(\tilde{\Omega})}\) because of Sobolev embedding and

$$\|\tilde{w}\|_{L^p(\tilde{\Omega})} \lesssim \|w\|_{L^p(\Omega)}.$$ \hspace{1cm} (3.4)

2. A priori \(W^2_p(\Omega)\)-estimate: If \(\tilde{w} \in W^2_{p,loc}(\tilde{\Omega}) \cap L^p(\tilde{\Omega})\) is a solution of (3.3), then we write (3.3) in nondivergence form

$$-\tilde{A} : D^2\tilde{w} - \text{div} \tilde{A} \cdot \nabla \tilde{w} = \tilde{f}$$

and apply the interior \(W^2_p\) estimates of [11 Theorem 9.11] to write

$$\|w\|_{W^2_p(\Omega)} = \|\tilde{w}\|_{W^2_p(\tilde{\Omega})} \lesssim \|\tilde{w}\|_{L^p(\tilde{\Omega})} + \|\tilde{f}\|_{L^p(\tilde{\Omega})} \lesssim \|w\|_{L^p(\Omega)} + \|f\|_{L^p(\Omega)}$$ \hspace{1cm} (3.5)

and \(w \in \hat{W}^1_2(\Omega)\). To show that this estimate implies (3.2), we argue by contradiction as in [7 Lemma 9.17]. Let \(\{w_m\} \subset W^2_p(\Omega) \cap \hat{W}^1_2(\Omega)\) be a sequence satisfying

$$\|w_m\|_{W^2_p(\Omega)} = 1, \quad \|f_m\|_{L^p(\Omega)} \to 0$$

as \(m \to \infty\), where \(f_m = -\text{div}(A\nabla w_m)\). Since the unit ball in \(W^2_p(\Omega)\) is weakly compact for \(1 < p < \infty\), there exists a subsequence, still labeled \(w_m\), that converges weakly in \(W^2_p(\Omega)\) and strongly in \(W^1_2(\Omega)\) to a function \(w \in W^2_p(\Omega) \cap W^1_2(\Omega)\). Therefore

$$\int_{\Omega} v f_m = -\int_{\Omega} v (A : D^2 w_m + \text{div} A \cdot \nabla w_m) \to -\int_{\Omega} v (A : D^2 w + \text{div} A \cdot \nabla w) = 0$$

for all \(v \in L^q(\Omega)\), whence \(-\text{div}(A\nabla w) = 0\) and \(w = 0\) because of uniqueness. On the other hand, (3.5) yields \(1 \lesssim \|w\|_{L^p(\Omega)}\), which is a contradiction. This thus shows the validity of (3.2).

3. Existence. It remains to show that there is a solution \(W^2_{p,loc}(\tilde{\Omega})\) of (3.3). If \(\tilde{f} \in L^2(\Omega)\), then the unique solution \(\tilde{w} \in H^1_0(\tilde{\Omega})\) of (3.3) belongs to \(H^2_{loc}(\tilde{\Omega})\) and

$$\|\tilde{w}\|_{H^2(\Omega')} \lesssim \|\tilde{w}\|_{H^1_0(\tilde{\Omega})} + \|\tilde{f}\|_{L^2(\tilde{\Omega})} \lesssim \|f\|_{L^2(\Omega)},$$

for all \(\Omega'\) compactly contained in \(\tilde{\Omega}\) [7 Theorem 8.8]. We first let \(p > 2\) and lift the regularity of \(\tilde{w}\) to \(W^2_p(\tilde{\Omega})\) upon applying [7 Lemma 9.16] which gives the estimate

$$\|\tilde{w}\|_{W^2_p(\Omega')} \lesssim \|\tilde{w}\|_{L^p(\tilde{\Omega})} + \|\tilde{f}\|_{L^p(\tilde{\Omega})}.$$ \hspace{1cm} (3.6)

If \(1 < p < 2\) instead, we approximate \(\tilde{f} \in L^p(\tilde{\Omega})\) by a sequence \(\{\tilde{f}_m\} \subset L^2(\tilde{\Omega})\). Since \(\tilde{w}_m \in H^2_{loc}(\tilde{\Omega}) \subset W^2_{p,loc}(\tilde{\Omega})\), we can apply the interior \(W^2_p\) estimates of [11 Theorem 9.11] to deduce (3.6) again for \(\tilde{w}_m\). Moreover, (3.6) shows that \(\{\tilde{w}_m\}\) is a Cauchy sequence in \(W^2_p(\Omega')\) for any \(\Omega'\), whence (3.6) remains valid for the limit \(w\). This finishes the proof. \(\square\)

3.2. State Equations. We resort to the fixed point argument in [11 Section 2] and [11 Section 4.1.1]. It consists of three steps: defining a convex set which acts as domain for the fixed point iterator, linearizing the free boundary problem by freezing one variable, and identifying conditions to guarantee a contraction on the convex set.
To deal with second-order regularity we need to introduce, besides the space $W^{1,1}_p$, the second order Banach subspace product

$$W^{2,2}_p := W^{1,1}_p \cap (W^2_p (0, 1) \times W^2_p (\Omega)),$$

and endow both $W^{1,1}_p$ and $W^{2,2}_p$ with the norms

$$\|(\gamma, y)\|_{W^{1,1}_p} := (1 + \beta C_A)|v|_{W^1_p(\Omega)}|y|_{W^1_p(0,1)} + |y|_{W^1_p(\Omega)}^2,$$

and

$$\|(\gamma, y)\|_{W^{2,2}_p} := (1 + 2 \beta C_A C_p)|v|_{W^2_p(\Omega)}^2 + |y|_{W^2_p(\Omega)}^2 + |y|_{W^2_p(0,1)}^2,$$

respectively; hereafter $C_A$ is a bound in $L^\infty(\Omega)$ on the operator $A$ and its first and second order derivatives $C_p$ respectively; hereafter $C_p$ is the constant in (3.2). To guarantee that the assumptions for the first-order regularity results in [1, Section 4.1.1] hold, we must iterate on a subset of [1, Eq. (4.12)]

$$\mathbb{B}_1 := \left\{(\gamma, y) \in W^{1,1}_\infty : |y|_{W^1_p(\Omega)} \leq \beta C_A |v|_{W^1_p(\Omega)}, |y|_{W^1_p(0,1)} \leq 1 \right\},$$

where $\beta$ is the inf-sup constant for $B_\Omega$ in $W^1_p(\Omega)$ [1, Proposition 4.1]. For the purpose of finding a strong solution, we further restrict $\mathbb{B}_1$ as follows:

$$\mathbb{B}_2 := \left\{(\gamma, y) \in \mathbb{B}_1 \cap W^{2,2}_\infty : |v|_{W^2_p(\Omega)} \leq 2 \beta C_A C_p |v|_{W^2_p(\Omega)}, |y|_{W^2_p(0,1)} \leq 1 \right\}.$$

We linearize the free boundary problem by considering the following operator $T : \mathbb{B}_2 \to W^{2,2}_\infty$ defined as

$$T(\gamma, y) := (T_1(\gamma, y), T_2(\gamma, y)) = (\tilde{\gamma}, \tilde{y}) \quad \forall (\gamma, y) \in \mathbb{B}_2,$$

where $\tilde{\gamma} = T_1(\gamma, y) = W^2_\infty (0, 1) \cap \tilde{W}^1_\infty (0, 1)$ is the unique solution to

$$- \kappa d^2_{1,1} \tilde{\gamma} = A[\gamma] \nabla(y + v) \cdot \nu + u \quad \text{in} \ (0, 1),$$

and $\tilde{y} = T_2(\gamma, y) = W^2_p (\Omega) \cap \tilde{W}^1_p (\Omega)$ is the unique solution to

$$- \text{div} \ (A [T_1(\gamma, y)] \nabla \tilde{y}) = \text{div} \ (A [T_1(\gamma, y)] \nabla v) \quad \text{in} \ \Omega,$$

where $\text{div} A [T_1(\gamma, y)]$ is computed row-wise. The operator $T$ maps $\mathbb{B}_1$ into itself provided $v$ and $u$ are restricted to verify

$$|v|_{W^2_p(\Omega)} \leq \frac{1 - \theta_1}{\alpha C \epsilon C_A (1 + \beta C_A)}, \quad \|u\|_{L^2(0,1)} \leq \frac{\theta_1}{\alpha},$$

for some $\theta_1 \in (\beta C_A/(1 + \beta C_A), 1)$ [1, Lemma 4.3]. We now investigate additional conditions for $T$ to map $\mathbb{B}_2$ into itself.

**Lemma 3.2** (range of $T$). *Let $C_S$ be the Sobolev embedding constant between $W^2_p (\Omega)$ and $W^1_\infty (\Omega)$. The operator $T$ maps $\mathbb{B}_2$ to $\mathbb{B}_2$ if, in addition to (3.10), the following relation holds

$$C_A C_S (1 + 2 \beta C_p) \|v\|_{W^2_p(\Omega)}^2 + \|u\|_{L^\infty(0,1)}^2 \leq \kappa.$$*
Proof. In view of (3.10) we have $T(B_2) \subset B_1$. Given $(\gamma, y) \in B_2$, we readily get from (3.8)

$$\kappa \|d_{x_1}^2 \gamma\|_{L^\infty(0,1)} \leq \|A[\gamma]\|_{L^\infty(0,1)} \|\nabla (y + v)\|_{L^\infty(\Omega)} + \|u\|_{L^\infty(0,1)}.$$

As $\|A[\gamma]\|_{L^\infty(0,1)} \leq C_A$, by definition of $C_A$, and for $p > 2$, $W^2_p(\Omega)$ is continuously embedded in $W^1_\infty(\Omega)$ with constant $C_S$, we deduce

$$\kappa \|d_{x_1}^2 \gamma\|_{L^\infty(0,1)} \leq C_A C_S \|y + v\|_{W^2_p(\Omega)} + \|u\|_{L^\infty(0,1)} \leq \kappa$$

because of (3.11). This implies $|\gamma|_{W^2_p(0,1)} \leq 1$, which is consistent with $B_2$.

To deal with (3.9), we invoke the a priori estimate (3.2) with $f = \text{div}(A[\gamma]\nabla v)$

$$\|\gamma\|_{W^2_p(\Omega)} \leq C\left(\|A[\gamma]\|_{L^\infty(\Omega)} \|v\|_{W^2_p(\Omega)} + \|\text{div} A[\gamma]\|_{L^\infty(\Omega)} |v|_{W^1_p(\Omega)}\right).$$

This gives

$$\|\gamma\|_{W^2_p(\Omega)} \leq 2C A C\|v\|_{W^2_p(\Omega)}.$$ 

and, together with the previous bound on $\gamma$, yields $(\gamma, y) \in B_2$, as asserted. \qed

Remark 3.3 (boundedness of $\bar{\gamma}$). We point out that, within the context of the optimal control problem, the $L^\infty$-estimate requirement on $\bar{u}$ in (3.11) can be satisfied. The reason is that the variational inequality (2.9) implies that

$$\Lambda = \kappa^{-1} C_A C_S (1 + 2C_A C\#)^2.$$

If, in addition to (3.10) and (3.11), the function $v$ further satisfies

$$\|v\|_{W^2_p(\Omega)} \leq (1 - \theta_2) \Lambda^{-1},$$

for some $\theta_2 \in (0, 1)$, then the map $T$ defined in (3.7) is a contraction on $B_2$ with constant $1 - \theta_2$ for all $u \in U_\text{ad}$.

Proof. Let $(\gamma_1, y_1), (\gamma_2, y_2) \in B_2$ with $(\gamma_1, y_1) \neq (\gamma_2, y_2)$, and set $\delta \gamma := \gamma_1 - \gamma_2$, $\delta y := y_1 - y_2$. Combining (3.7) and (3.8) we get an equation for $\delta \gamma := \gamma_1 - \gamma_2$

$$-\kappa d_{x_1}^2 \delta \gamma = (A[\gamma_1] - A[\gamma_2]) \nabla (y_1 + v) \cdot \nu + A[\gamma_2] \nabla \delta y \cdot \nu.$$ 

Since $\delta \gamma(0) = \delta \gamma(1) = 0$ we infer that $\delta \gamma'(x_1) = 0$ for some $x_1 \in (0, 1)$ and $|\delta \gamma|_{W^2_p(0,1)} \leq |\delta \gamma|_{W^2_p(0,1)}$, whence

$$\|\delta \gamma\|_{W^2_p(0,1)} \leq C_A C_S \|\delta \gamma, \delta y\|_{W^2_p(0,1)} \leq \kappa^{-1} C_A C_S (\delta \gamma, \delta y)_{W^2_p(0,1)}.$$
We next estimate $\delta \tilde{y} := \tilde{y}_1 - \tilde{y}_2$. In view of (3.9), we see that
\[-\text{div} \left( A [\bar{\gamma}] \nabla \delta \tilde{y} \right) = \text{div} \left( (A [\bar{\gamma}]_1 - A [\bar{\gamma}]_2) \nabla (\tilde{y}_2 + v) \right).\]
Invoking the a priori estimate (3.2), we deduce
\[
\|\delta \tilde{y}\|_{W^2_p(\Omega)} \leq C\# \|A [\bar{\gamma}]_1 - A [\bar{\gamma}]_2\|_{L^\infty(0,1)} \|\tilde{y}_2 + v\|_{W^2_p(\Omega)} \nabla \delta \gamma, \delta \gamma y \\text{and, applying } (3.13), \text{we obtain}
\[
\|\delta \tilde{y}\|_{W^2_p(\Omega)} \leq 2C\# \|A [\bar{\gamma}]_1 - A [\bar{\gamma}]_2\|_{L^\infty(0,1)} \|\tilde{y}_2 + v\|_{W^2_p(\Omega)}.
\]
Since $\|\tilde{y}_2\|_{W^2_p(\Omega)} \leq 2C\# \|v\|_{W^2_p(\Omega)}$, we infer that
\[
\|\delta \tilde{y}\|_{W^2_p(\Omega)} \leq 2C\# \left( 1 + 2C\# \|\tilde{y}\|_{W^2_p(\Omega)} \right) \|\delta \gamma\|_{W^2_p(\Omega)}.
\]
and, applying (3.13), we obtain
\[
\|\delta \tilde{y}\|_{W^2_p(\Omega)} \leq 2\kappa^{-1} C^2_2 C\# \left( 1 + 2C\# \|\tilde{y}\|_{W^2_p(\Omega)} \right) \|\delta \gamma\|_{W^2_p(\Omega)}.
\]
The definition of $W^{2,2}_{k,p}$ norm, together with (3.13) and (3.14), leads to
\[
\|\delta \gamma, \delta \gamma y \|_{W^{2,2}_{k,p}} \leq \kappa^{-1} C\# C S \left( 1 + 2C\# \|\tilde{y}\|_{W^2_p(\Omega)} \right) \|\delta \gamma, \delta \gamma y \|_{W^{2,2}_{k,p}}.
\]
and (3.12) gives $\|\delta \gamma, \delta \gamma y \|_{W^{2,2}_{k,p}} \leq \theta_2 \|\delta \gamma, \delta \gamma y \|_{W^{2,2}_{k,p}}$, which is the assertion. \(\Box\)

### 3.3. Adjoint Equations.
We begin by assuming that $(\bar{\gamma}, \tilde{y})$ belongs to $B_2$ and rewriting the adjoint equations (2.10) in strong divergence form in $\Omega$
\[-\text{div} \left( A [\bar{\gamma}] \nabla \bar{\gamma} \right) = \delta \tilde{y} (1 + \bar{\gamma}),
\]
and in (0, 1)
\[-\kappa d_{x_1} \bar{s} = \delta \bar{\gamma} + \frac{1}{2} \int_0^1 |\delta \tilde{y}|^2 \text{d}x_2
\]
\[-\int_0^1 A_1 [\bar{\gamma}] \nabla (\tilde{y} + v) \cdot \nabla \bar{\gamma} \text{d}x_2 + \int_0^1 A_2 [\bar{\gamma}] \nabla (\tilde{y} + v) \cdot \nabla \bar{\gamma} \text{d}x_2
\]
together with the boundary conditions $\bar{\gamma} = 0$ on $\Sigma$, $\bar{\gamma} = \tilde{s}$ on $\Gamma$, and $\bar{s}(0) = \bar{s}(1) = 0$.

**Theorem 3.5** (second-order regularity of adjoint variables). The solution $(\bar{s}, \bar{\gamma})$ to (3.15) satisfies $(\bar{s}, \bar{\gamma} - ES) \in W^{2,q}_{1,q}$ along with the following a-priori estimates
\[
\|\bar{s}\|_{W^2_{p,1}(0,1)} + \|\bar{\gamma}\|_{W^2_{p,1}(0)} \leq \|\delta \gamma\|_{L^2(0,1)} + \|\delta \tilde{y}\|_{L^2(0,1)} + \|\delta \tilde{y}\|_{L^2(0,1)}
\]
provided the function $v$ satisfies
\[
4C\# C E (1 + 2C\#) \left( 2(1 + 2C\# C\#) + \alpha (1 + \beta C\#) \right) \|v\|_{W^2_p(\Omega)} \leq 1.
\]

**Proof.** Setting $\bar{r} = \bar{r}_0 + E \bar{s}$, where $E : W^2_{q,1}(0,1) \cap W^1_{q,1}(0,1) \to W^2_{q,1}(\Omega)$ is the extension operator for $q < 2$, we can rewrite (3.15a) as
\[-\text{div} \left( A [\bar{\gamma}] \nabla \bar{r}_0 \right) = \text{div} \left( A [\bar{\gamma}] \nabla E \bar{s} \right) + \delta \tilde{y} (1 + \bar{\gamma}),
\]
with \( \bar{r}_0 | \partial \Omega = 0 \). We apply \( 32 \) to obtain \( \bar{r}_0 \in W^2_2(\Omega) \) and
\[
\| \bar{r}_0 \|_{W^2_2(\Omega)} \leq 2C\| \bar{s} \|_{W^2_2(\Omega)} \left. + 2C\| \delta \bar{y} \|_{L^2(\Omega)}, \right.
\]
and similarly for \( \bar{s} \)
\[
\| \bar{s} \|_{W^2_2(\Omega)} \leq \| \delta \bar{y} \|_{L^2(\Omega)} + \frac{1}{2} \| \delta \bar{y} \|_{L^2(\Omega)}^2 + 4CA\| \delta \bar{y} \| + v\| \bar{y} \|_{W^1_2(\Omega)} \| \bar{r} \|_{W^1_2(\Omega)}.
\]
Using the fact \( \bar{y} \in B_2 \) we deduce
\[
\| \bar{s} \|_{W^2_2(\Omega)} \leq \| \delta \bar{y} \|_{L^2(\Omega)} + \frac{1}{2} \| \delta \bar{y} \|_{L^2(\Omega)}^2 + 4CA \left( 1 + 2CA\| \bar{s} \|_{W^1_2(\Omega)} \right) \| \bar{r} \|_{W^1_2(\Omega)}.
\]
Recalling the estimate for \( |\bar{s}|_{W^1_2(\Omega)} \) from \( 11 \) Lemma 5.5
\[
|\bar{s}|_{W^1_2(\Omega)} \leq \alpha\| \delta \bar{y} \|_{L^1(\Omega)} + \frac{\alpha}{2} \| \delta \bar{y} \|_{L^2(\Omega)} + \alpha CA \left( 1 + \beta CA \right) |\bar{v}|_{W^1_2(\Omega)} |\bar{r}|_{W^1_2(\Omega)},
\]
and using that \( |\bar{s}|_{L^1(\Omega)} \leq |\bar{s}|_{W^1_2(\Omega)} \), we end up with
\[
|\bar{s}|_{W^2_2(\Omega)} \leq \left( 1 + 2\alpha \right) \| \delta \bar{y} \|_{L^1(\Omega)} + \frac{1}{2} \left( 1 + 2\alpha \right) \| \delta \bar{y} \|_{L^2(\Omega)}^2 + \lambda \| \bar{v} \|_{W^1_2(\Omega)} \| \bar{r} \|_{W^1_2(\Omega)},
\]
where \( \lambda = 2CA \left( 1 + 2CA\| \bar{s} \|_{W^1_2(\Omega)} + \alpha \left( 1 + \beta CA \right) \right) \). Inserting the estimate for \( \| \bar{r}_0 \|_{W^2_2(\Omega)} \) into this estimate, we get
\[
|\bar{s}|_{W^2_2(\Omega)} \leq \left( 1 + 2\alpha \right) \| \delta \bar{y} \|_{L^1(\Omega)} + \frac{1}{2} \left( 1 + 2\alpha \right) \| \delta \bar{y} \|_{L^2(\Omega)}^2 + \lambda \| \bar{v} \|_{W^1_2(\Omega)} \| \bar{s} \|_{W^1_2(\Omega)} + 2\lambda C\| \delta \bar{y} \|_{L^2(\Omega)} \| \bar{r} \|_{W^1_2(\Omega)}
\]
and the desired estimate for \( |\bar{s}|_{W^2_2(\Omega)} \) follows from \( 3.16 \). This, and the relation \( \bar{r} = \bar{r}_0 + E\bar{s} \) yields the remaining estimate for \( \| \bar{r} \|_{W^2_2(\Omega)} \), and concludes the proof. \( \Box \)

4. Discrete Optimal Control Problem. The goal of this section is to introduce the discrete counterpart of the optimization problem \( 2.5 \). The discretization uses the finite element method and is classical.

Let \( T \) denote a geometrically conforming rectangular quasi-uniform triangulation of the fixed domain \( \Omega \) such that \( \Omega = \bigcup_{K \in T} K \) and \( h \approx h_K \) be the meshsize of \( T \). Additionally, let \( 0 = \zeta_0 < \zeta_1 < \ldots < \zeta_{M+1} = 1 \) be a partition of \( [0,1] \) with nodes \( \zeta_i \) compatible with \( T \). Consider the following finite dimensional spaces, where the capital letters stand for discrete objects:
\[
\forall h := \left\{ Y \in C^0(\bar{\Omega}) : Y|_{K} \in \mathcal{P}^1(K), K \in T \right\}, \quad (4.1a)
\]
\[
\forall f := \forall h \cap W^1_p(\Omega), \quad (4.1b)
\]
\[
\mathcal{S}_h := \left\{ G \in C^0([0,1]) : G|_{[\zeta_i, \zeta_{i+1}]} \in \mathcal{P}^1([\zeta_i, \zeta_{i+1}]), \ 0 \leq i \leq M \right\}, \quad (4.1c)
\]
\[
\tilde{\mathcal{S}}_h := \mathcal{S}_h \cap W^1_\infty(0,1), \quad (4.1d)
\]
\[
U_{ad} := \tilde{\mathcal{S}}_h \cup U_{ad}, \quad (4.1e)
\]
and \( \mathcal{P}^1(D) \) stands for bilinear polynomials on an element \( D = K \in T \) or linear polynomials on an interval \( D = [\zeta_i, \zeta_{i+1}] \). The spaces \( \forall h, \mathcal{S}_h \) and \( U_{ad} \) in \( 4.1 \) will be
used to approximate the continuous solutions \((y, \gamma, u)\) of \((2.5)\). This discretization is classical [1], Chapter 3, except perhaps for the \(L^2\) constraint in \(\mathbb{U}_{ad}\), which we enforce by scaling the functions with their \(L^2\)-norm; for more details we refer to Section 7.

Next we present a discrete analog of the continuous extension \((2.3)\), namely

\[
E_h G := (S_h \circ E)(G), \quad \forall G \in \hat{S}_h.
\]

The caveat is that functions in \(W^1_p(\Omega)\) are not necessarily continuous. This issue is addressed by utilizing the Scott-Zhang interpolation operator \(S_h : W^1_q(\Omega) \to \mathbb{V}_h\). This operator satisfies the optimal estimate [4],

\[
|w - S_h w|_{W^1_q(\Omega)} \lesssim h|w|_{W^2_q(\Omega)}, \quad \forall w \in W^2_q(\Omega), \quad 1 \leq q \leq \infty.
\] (4.2)

For functions in \(W^1_q(\Omega)\) with \(p > 2\), \(W^1_q(0,1)\) and \(W^1_1(0,1)\) we will use the standard Lagrange interpolation operator \(I_h\). This is justified by the Sobolev embedding theorems, i.e. we can identify functions in those spaces with their continuous equivalents. Moreover, the following optimal interpolation estimates hold,

\[
|y - I_h y|_{W^1_q(\Omega)} \lesssim h|y|_{W^2_q(\Omega)}, \quad \forall y \in W^2_q(\Omega), \quad 2 < p \leq \infty,
\] (4.3a)

\[
|\gamma - I_h \gamma|_{W^1_q(0,1)} \lesssim h|\gamma|_{W^2_q(0,1)}, \quad \forall \gamma \in W^2_q(0,1), \quad 1 \leq p \leq \infty.
\] (4.3b)

Next we state the discrete counterpart of the optimal control problem \((2.5)\) in its variational form: if \(\delta G := G - \gamma_d\), \(\delta Y := Y + v - y_d\), then minimize

\[
J_h(G,Y,U) := \frac{1}{2} \|\delta G\|^2_{L^2(\Omega)} + \frac{1}{2} \|\delta Y \sqrt{I+G}\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|U\|^2_{L^2(\Omega)},
\] (4.4a)

subject to the discrete state equation \((G,Y) \in \hat{S}_h \times \hat{V}_h\)

\[
\begin{align*}
\mathcal{B}_T[G,\Xi] + \mathcal{B}_\Omega[Y + v, Z + E_h \Xi; A[G]] &= \int_0^1 U \Xi \quad \forall (\Xi,Z) \in \hat{S}_h \times \hat{V}_h, \quad (4.4b)
\end{align*}
\]

the state constraints

\[
|G'| \leq 1 \quad \text{on } (\zeta_i, \zeta_{i+1}), \quad i = 0, \ldots, M - 1,
\] (4.4c)

and the control constraints

\[
U \in \mathbb{U}_{ad}.
\]

We point out that \(Y|_{\partial \Omega} = 0\) in (4.4b). This is not the standard approach in finite element literature because it requires knowing an extension of \(v\) to \(\Omega\); we adopt this approach to simplify the exposition. We must include the following mild regularity assumptions on data in order to obtain an order of convergence:

(A_3) The given data satisfy \(v \in W^2_p(\Omega), \gamma_d \in L^2(0,1)\) and \(y_d \in L^2(\Omega^*)\).

Now let \(\bar{U}\) denote the optimal control to \((4.4a)\), whose existence will be shown in Theorem 4.2. Let \((\bar{G}, \bar{Y})\) be the optimal state, which satisfy discrete state equations in variational form \((4.4b)\). The discrete adjoint equations in variational form read: find \((\hat{S}, \hat{R})\) such that \((\hat{S}, \hat{R} - E_h \hat{S}) \in \hat{S}_h \times \hat{V}_h\) and for every \((\Xi,Z) \in \hat{S}_h \times \hat{V}_h\),

\[
\mathcal{B}_T[\Xi, \hat{S}] + \mathcal{D}_\Omega[\Xi, Z, \hat{R}; \bar{G}, \bar{Y}] = \left\langle \Xi, \delta \hat{G} + \frac{1}{2} \int_0^1 |\delta \bar{Y}|^2 \, dx_2 \right\rangle + \left\langle Z, \delta \bar{Y} (1 + \bar{G}) \right\rangle.
\] (4.5)
Finally, the optimal control $\bar{U}$ satisfies the variational inequality

$$\langle \mathcal{J}_h'(\bar{U}), U - \bar{U} \rangle_{L^2(0,1) \times L^2(0,1)} \geq 0 \quad \forall U \in \mathcal{U}_{ad},$$

(4.6)

where $\mathcal{J}_h'(\bar{U}) = \dot{S} + \lambda \bar{U}$. Therefore (4.6) reads

$$\langle \dot{S} + \lambda \bar{U}, U - \bar{U} \rangle_{L^2(0,1) \times L^2(0,1)} \geq 0 \quad \forall U \in \mathcal{U}_{ad}.$$  

(4.7)

The following discrete estimates mimic the continuous inf-sup $[1]$ Proposition 4.1.

**PROPOSITION 4.1** (discrete inf-sup). The following two statements hold:

(i) There exists constant $0 < \alpha < \infty$ independent of $h$ such that

$$|G|_{W^1_0(\Omega)} \leq \alpha \sup_{0 \neq \Xi \in \mathcal{S}_h} \frac{B_F[G, 

\Xi]}{|\Xi|_{W^1_0(\Omega)}},$$

(4.8a)

$$|S|_{W^1_0(\Omega)} \leq \alpha \sup_{0 \neq \Xi \in \mathcal{S}_h} \frac{B_F[\Xi, S]}{|\Xi|_{W^1_0(\Omega)}}. $$

(4.8b)

(ii) There exists constant $0 < \beta < \infty$ independent of $h$ and constants $Q < 2 < P$, $h_0 > 0$, such that for $p \in [Q, P]$ and $0 < h \leq h_0$

$$|Y|_{W^1_0(\Omega)} \leq \beta \sup_{0 \neq Z \in \mathcal{V}_h} \frac{B_\Omega \left[ Y, Z; A[G] \right]}{|Z|_{W^1_0(\Omega)}}.$$ 

(4.9)

**Proof.** We refer to $[11]$ Proposition 3.2 for a proof of (4.8a) and to $[1]$ Proposition 8.6.2 for a proof of (4.9). The technique of $[11]$ extends to (4.8b). □

Existence and uniqueness of solutions to the state and adjoint equations can be shown similarly to the continuous case $[1]$ Corollary 4.6, and Theorem 5.6] provided $U \in \mathcal{U}_{ad}$ and $|v|_{W^1_0(\Omega)}$ is small. We will next prove existence of an optimal control $\bar{U}$ solving (4.4a).

**THEOREM 4.2** (existence of optimal control). There exists a discrete optimal control $\bar{U} \in \mathcal{U}_{ad}$ which solves (4.4a).

**Proof.** The proof follows by using a minimizing sequence argument similar to the continuous proof $[1]$ Theorem 5.1. However, weak convergence of a minimizing sequence $\{U_n\}$ yields strong convergence in finite dimensional spaces. Following $[1]$ Theorem 4.8] it is routine to show that the discrete control-to-state map is Lipschitz continuous. Together with this Lipschitz continuity and the strong convergence of $U_n$, we also obtain strong convergence of the associated state sequence $\{(G_n, Y_n)\}$. □

**5. A-priori Error Estimates: State and Adjoint Variables.** The goal of this section is to derive a-priori error estimates between the continuous and discrete solutions of the state and adjoint equations for given functions $u \in \mathcal{U}_{ad}$ and $U \in \mathcal{U}_{ad}$. This is the content of Lemmas 5.1 through 5.6. These estimates are the stepping stone for the $L^2$ estimate of $\bar{U} - U$ in Theorem 6.1.

**LEMMA 5.1** (preliminary error estimate for $\gamma$). Given $u \in \mathcal{U}_{ad}$ and $U \in \mathcal{U}_{ad}$, let $(\gamma, y)$ and $(G, Y)$ solve (2.5b) and (4.4b) respectively for $v \in W^2_0(\Omega)$ with $|v|_{W^1_0(\Omega)}$ small. Then the following error estimate for $\gamma - G$ holds

$$|\gamma - G|_{W^1_0(\Omega)} \leq h |\gamma|_{W^2_0(\Omega)} + |y - Y|_{W^1_0(\Omega)} + \|u - U\|_{L^2(0,1)}.$$
Proof. We use the discrete inf-sup \((4.8a)\) to infer that

\[
|\mathcal{I}_h \gamma - G|_{W^1_p(\Omega)} \lesssim \sup_{0 \neq \Xi \in \mathcal{S}_h} \frac{B_T [I_h \gamma - G, \Xi]}{\|\Xi\|_{W^1_p(\Omega)}}.
\]

Next, we rewrite \(B_T [I_h \gamma - G, \Xi] = B_T [I_h \gamma - \gamma, \Xi] + B_T [\gamma - G, \Xi]\), and estimate the first term using Hölder’s inequality and \((4.3b)\). For the second term we set \(w = y + v\) and \(W = Y + v\), use that \(\gamma\) and \(G\) satisfy \((2.5b)\) and \((4.4b)\) respectively, and the fact that \(|y|_{W^1_p(\Omega)} \lesssim |v|_{W^1_p(\Omega)}\), to obtain

\[
B_T [\gamma - G, \Xi] = -B_\Omega [w, E_h \Xi; A [\gamma]] + B_\Omega [W, E_h \Xi; A [G]] + \langle u - U, \Xi \rangle \\
= B_\Omega [w, E_h \Xi; A [\gamma] + A [G]] + B_\Omega [W - w, E_h \Xi; A [G]] + \langle u - U, \Xi \rangle \\
\lesssim (|\gamma - G|_{W^1_p(\Omega)} |v|_{W^1_p(\Omega)} + |y - Y|_{W^1_p(\Omega)} + \|u - U\|_{L^2(\Omega)}) |\Xi|_{W^1_p(\Omega)},
\]

where \(\langle u - U, \Xi \rangle = \langle u - U, \Xi \rangle_{L^2(\Omega) \times L^2(\Omega)}\). Combining the above two estimates with the triangle inequality and \((4.3b)\), we end up with

\[
|\gamma - G|_{W^1_p(\Omega)} \lesssim \|v|_{W^1_p(\Omega)} + |y - Y|_{W^1_p(\Omega)} + \|u - U\|_{L^2(\Omega)}.
\]

Using that \(|v|_{W^1_p(\Omega)}\) is small finally yields the desired result. \(\square\)

**Lemma 5.2** (error estimate for \(y\)). Given \(u \in U_{ad}\) and \(U \in U_{ad}\), let \((\gamma, y)\) and \((G, Y)\) solve \((2.5b)\) and \((4.4b)\) respectively with \(|v|_{W^1_p(\Omega)}\) small. Then the following estimate for \(y - Y\) holds

\[
|y - Y|_{W^1_p(\Omega)} \lesssim h \left( |\gamma|_{W^1_p(\Omega)} + |y|_{W^1_p(\Omega)} \right) + |v|_{W^1_p(\Omega)} \|u - U\|_{L^2(\Omega)}.
\]

Proof. We proceed as in Lemma 5.1. We use the discrete inf-sup followed by the interpolation estimate \((4.3a)\), together with the state constraint \(|G|_{W^1_p(\Omega)} \leq 1\), to obtain

\[
|\mathcal{I}_h y - Y|_{W^1_p(\Omega)} \lesssim \sup_{0 \neq Z \in \mathcal{V}_h} \frac{B_\Omega [\mathcal{I}_h y - Y, Z; A [G]]}{|Z|_{W^1_p(\Omega)}} \\
\lesssim h |y|_{W^1_p(\Omega)} + \sup_{0 \neq Z \in \mathcal{V}_h} \frac{B_\Omega [y - Y, Z; A [G]]}{|Z|_{W^1_p(\Omega)}}.
\]

We handle the last term by using that \(y\) and \(Y\) are solutions to \((2.5b)\) and \((4.4b)\), i.e.

\[
B_\Omega [y - Y, Z; A [G]] = B_\Omega [y + v, Z; A [G]] - B_\Omega [y + v, Z; A [G]] \\
= B_\Omega [y + v, Z; A [G] - A [\gamma]],
\]

followed by the bound \(|y|_{W^1_p(\Omega)} \lesssim |v|_{W^1_p(\Omega)}\) in the definition of \(\mathcal{B}_1\) to yield

\[
B_\Omega [y - Y, Z; A [G]] \lesssim |\gamma - G|_{W^1_p(\Omega)} |v|_{W^1_p(\Omega)} |Z|_{W^1_p(\Omega)}.
\]
Combining the above estimates with Lemma 5.1 and using the triangle inequality in conjunction with (4.3a), we obtain

\[
|y - Y|_{W^1_2(\Omega)} \lesssim h|y|_{W^1_2(\Omega)} + |\gamma - G|_{W^1_2(0,1)}|v|_{W^1_2(\Omega)}
\]

\[
\lesssim h \left( |\gamma|_{W^1_2(0,1)}|v|_{W^1_2(\Omega)} + |y|_{W^1_2(\Omega)} \right) + \|u - U\|_{L^2(0,1)}|v|_{W^1_2(\Omega)} + |y - Y|_{W^1_2(\Omega)}|v|_{W^1_2(\Omega)}.
\]

The desired estimate is a consequence of the smallness assumption on $|v|_{W^1_2(\Omega)}$. □

**Lemma 5.3** (error estimate for $\gamma$). Given $u \in U_{ad}$ and $U \in U_{ad}$, let $(\gamma, y)$ and $(G, Y)$ solve (2.5b) and (4.4b) respectively with $|v|_{W^1_2(\Omega)}$ small. Then the following error estimate for $\gamma - G$ holds

\[
|\gamma - G|_{W^1_2(0,1)} \lesssim h \left( |\gamma|_{W^1_2(0,1)} + |y|_{W^1_2(\Omega)} \right) + \|u - U\|_{L^2(0,1)}.
\]

**Proof.** The assertion follows by combining Lemma 5.2 with Lemma 5.1. □

**Lemma 5.4** (preliminary error estimate for $s$). Given $u \in U_{ad}$ and $U \in U_{ad}$, let $(s, r - E_h S) \in W^1_2(0,1) \times W^1_2(\Omega)$ satisfy the continuous adjoint system (2.10), and $(S, R - E_h S) \in \tilde{S}_h \times \tilde{V}_h$ satisfy the discrete counterpart (4.5). Then the following error estimate for $s - S$ is valid

\[
|s - S|_{W^1_2(0,1)} \lesssim h|s|_{W^1_2(0,1)} + \left( 1 + |r|_{W^1_2(\Omega)}|v|_{W^1_2(\Omega)} \right) |\gamma - G|_{W^1_2(0,1)}
\]

\[
+ \left( |\delta y|_{L^2(\Omega)} + |y - Y|_{W^1_2(\Omega)} + |r|_{W^1_2(\Omega)} \right) |y - Y|_{W^1_2(\Omega)} + |r - R|_{W^1_2(\Omega)}|v|_{W^1_2(\Omega)}.
\]

**Proof.** We again employ the discrete inf-sup (4.8b), now taking the form

\[
|I_h s - S|_{W^1_2(0,1)} \lesssim \sup_{0 \neq \Xi \in \tilde{S}_h} \frac{\mathcal{B}_r \left[ \Xi, I_h s - S \right]}{|\Xi|_{W^1_2(0,1)}}
\]

\[
\lesssim h|s|_{W^1_2(0,1)} + \sup_{0 \neq \Xi \in \tilde{S}_h} \frac{\mathcal{B}_r \left[ \Xi, s - S \right]}{|\Xi|_{W^1_2(0,1)}},
\]

where the last inequality follows by adding and subtracting $s$, the continuity of $\mathcal{B}_r$, and the interpolation estimate (4.3b) for $s - I_h s$. It remains to control the last term. We use that $s$ and $S$ satisfy equations (2.10) and (4.5) to obtain

\[
\mathcal{B}_r \left[ \Xi, s - S \right] = \langle \Xi, \gamma - \gamma_d \rangle - \langle \Xi, G - \gamma_d \rangle
\]

\[
+ \left( \Xi, \frac{1}{2} \int_0^1 |y + v - y_d|^2 \, dx_2 \right) - \left( \Xi, \frac{1}{2} \int_0^1 |Y + v - y_d|^2 \, dx_2 \right)
\]

\[- \mathcal{B}_\Omega \left[ y + v, r; DA \left[ \gamma \right] \langle \Xi \rangle \right] + \mathcal{B}_\Omega \left[ Y + v, r; DA \left[ G \right] \langle \Xi \rangle \right]
\]

\[= \langle \Xi, \gamma - G \rangle + \left( \Xi, \frac{1}{2} \int_0^1 (y - Y) (y + Y + 2v - 2y_d) \, dx_2 \right)
\]

\[- \mathcal{B}_\Omega \left[ y - Y, r; DA \left[ \gamma \right] \langle \Xi \rangle \right] - \mathcal{B}_\Omega \left[ Y + v, r; DA \left[ \gamma - DA \left[ G \right] \right] \langle \Xi \rangle \right]
\]

\[- \mathcal{B}_\Omega \left[ Y + v, r - R; DA \left[ G \right] \langle \Xi \rangle \right].
\]
Consequently, after normalization $|\Xi|_{W^{1,1}_0(\Omega)} = 1$, we infer that
\[
|B_{\Omega} [\Xi, s - S]| \lesssim \|\gamma - G\|_{L^1(\Omega)} + \|y - Y\|_{L^2(\Omega)} \left( 2\|y + v - y_d\| + \|Y - y\|_{L^2(\Omega)} \right) + |y - Y|_{W^1_p(\Omega)} |r|_{W^1_0(\Omega)} + |v|_{W^1_p(\Omega)} \left( |r|_{W^1_0(\Omega)} \|\gamma - G\|_{W^{1,1}_0(\Omega)} + |r - R|_{W^1_0(\Omega)} \right).
\]
The desired result for $|I_h s - S|_{W^1_0(\Omega)}$ follows after combining the above estimate with $\|\gamma - G\|_{L^1(\Omega)} \lesssim |\gamma - G|_{W^{1,1}_0(\Omega)}$ and $\|y - Y\|_{L^2(\Omega)} \lesssim |y - Y|_{W^1_0(\Omega)}$. Finally, applying the triangle inequality in conjunction with (4.3b) we deduce the asserted estimate for $|s - S|_{W^1_0(\Omega)}$.

**Lemma 5.5 (error estimate for $r$).** Given $u \in U_{ad}$ and $U \in U_{ad}$, let $(s, r - Es) \in W^1_0(0, 1) \times W^1_p(\Omega)$ satisfy the continuous adjoint system (2.10), and $(S, R - EhS) \in \hat{S}_h \times \hat{\nu}_h$ satisfy the discrete counterpart (4.5). Then the following a-priori error estimate for $r - R$ holds
\[
|r - R|_{W^1_0(\Omega)} \lesssim h \left( |s|_{W^1_0(\Omega)} + |r|_{W^1_0(\Omega)} \right) + \left( 1 + (1 + |v|_{W^1_0(\Omega)} \|r|_{W^1_0(\Omega)} + \|\delta y\|_{L^\infty(\Omega)} \right) |\gamma - G|_{W^{1,1}_0(\Omega)} + |y - Y|_{W^1_0(\Omega)} + |r|_{W^1_0(\Omega)} \right) |y - Y|_{W^1_0(\Omega)}.
\]

**Proof.** Since the discrete inf-sup (4.9) is for functions in $\hat{\nu}_h$, we write $r = r_0 + Es$, and $R = R_0 + EhS$, with $r_0 \in W^1_0(\Omega)$ and $R_0 \in \hat{\nu}_h$, to obtain
\[
|r - R|_{W^1_0(\Omega)} \leq |r_0 - S_h r_0|_{W^1_0(\Omega)} + |S_h r_0 - R_0|_{W^1_0(\Omega)} + |Es - EhS|_{W^1_0(\Omega)}.
\]
Consequently, applying (4.9)
\[
|S_h r_0 - R_0|_{W^1_0(\Omega)} \lesssim h |r_0|_{W^1_0(\Omega)} + \sup_{0 \neq Z \in \hat{\nu}_h} \frac{B_{\Omega} [Z, r_0 - R_0; A[G]]}{|Z|_{W^1_0(\Omega)}},
\]
where we have added and subtracted $r_0$. Moreover, we handle the last term as before, i.e.
\[
B_{\Omega} [Z, r_0 - R_0; A[G]] = B_{\Omega} [Z, r_0 + Es; A[\gamma]] - B_{\Omega} [Z, R_0 + EhS; A[G]] + B_{\Omega} [Z, r_0 + Es; A[G] - A[\gamma]] + B_{\Omega} [Z, EhS - Es; A[G]].
\]
Invoking the adjoint equations (2.10) and (4.5), we see that
\[
B_{\Omega} [Z, r_0 + Es; A[\gamma]] - B_{\Omega} [Z, R_0 + EhS; A[G]] = \langle (y + v - y_d)(1 + \gamma), Z \rangle - \langle (Y + v - y_d)(1 + G), Z \rangle = \langle y - Y, Z \rangle + \langle y - y_d(G - \gamma), Z \rangle.
\]
Since $y\gamma - YG = y(\gamma - G) - (Y - y)G$, after normalization $|Z|_{W^1_p(\Omega)} = 1$ and using (4.4c), we obtain
\[
|B_{\Omega} [Z, r_0 - R_0; A[G]]| \lesssim \|y - Y\|_{L^\infty(\Omega)} + |\gamma - G|_{W^{1,1}_0(\Omega)} \left( |r|_{W^1_0(\Omega)} + \|\delta y\|_{L^\infty(\Omega)} \right) + |Es - EhS|_{W^1_0(\Omega)}.
\]
The assertion follows by applying Lemmas 5.2 and 5.3, together with (4.6). Since \( \bar{r} \) and on the continuous and discrete first-order optimality conditions (2.9) and discrete adjoint equation (4.5) solutions of the state equation (2.5b) exist. Finally, under the smallness assumption on \( v \) the smallness assumption on \( v \) the smallness assumption on \( v \) the smallness assumption on \( v \) and \( y \) we end up with

\[
|s - \bar{r}|_{W^1_p(\Omega)} \lesssim h \left( |s|_{W^1_p(\Omega)} + |r|_{W^1_p(\Omega)} \right) + \|y - Y\|_{L^\infty(\Omega)} + \|G\|_{W^{1,p}_\infty(\Omega)} + \|\delta y\|_{L^2(\Omega)} + |s|_{W^1_p(\Omega)} + |r|_{W^1_p(\Omega)} + \|u - U\|_{L^2(\Omega)}.
\]

**Proof.** We use Lemmas 5.4 and 5.5 to obtain

\[
|s - \bar{r}|_{W^1_p(\Omega)} \lesssim h \left( |s|_{W^1_p(\Omega)} + |v|_{W^1_p(\Omega)} \left( |s|_{W^1_p(\Omega)} + |r|_{W^1_p(\Omega)} \right) \right) + \left( c_1 + |v|_{W^1_p(\Omega)} \left( c_1 + c_3 \right) \right) \gamma - G|_{W^{1,p}_\infty(\Omega)} + \left( c_2 + |y - Y|_{W^1_p(\Omega)} + |v|_{W^1_p(\Omega)} \left( 1 + c_2 + |y - Y|_{W^1_p(\Omega)} \right) \right) |y - Y|_{W^1_p(\Omega)}
\]

where

\[
c_1 = 1 + |r|_{W^1_p(\Omega)}|v|_{W^1_p(\Omega)},
\]

\[
c_2 = |r|_{W^1_p(\Omega)} + \|\delta y\|_{L^2(\Omega)},
\]

\[
c_3 = |r|_{W^1_p(\Omega)} + \|\delta y\|_{L^2(\Omega)}.
\]

The assertion follows by applying Lemmas 5.2 and 5.3, together with \( |v|_{W^1_p(\Omega)} \leq 1 \).

**6. A-priori Error Estimates: Optimal Control.** Next we derive the a-priori error estimate for \( u \) and \( \bar{U} \).

**Theorem 6.1 (error estimate for \( u \)).** Let both \( h_0 \) and \( |v|_{W^1_p(\Omega)} \) be sufficiently small. If \( h \leq h_0 \), then

\[
\|\bar{u} - \bar{U}\|_{L^2(\Omega)} \leq \frac{4}{\lambda} \|s(\bar{U}) - S(\bar{U})\|_{L^2(\Omega)},
\]

where \( s(\bar{U}) \) is the solution of the continuous adjoint equation (2.10) with \( (\bar{U}, y(\bar{U})) \) solutions of the state equation (2.5b) with control \( U \), and \( S(\bar{U}) \) is the solution of the discrete adjoint equation (4.5).

**Proof.** The proof relies primarily on the continuous quadratic growth condition (2.18) and on the continuous and discrete first-order optimality conditions (2.9) and (4.6). Since \( \bar{U} \in \mathcal{U}_{ad} \) is admissible, according to (4.1), replacing \( u \) by \( \bar{U} \) in (2.18) we get

\[
\frac{\lambda}{4} \|\bar{U} - \bar{u}\|_{L^2(\Omega)}^2 \leq \langle \mathcal{J}'(\bar{U}) - \mathcal{J}'(\bar{u}), \bar{U} - \bar{u}\rangle_{L^2(\Omega) \times L^2(\Omega)},
\]

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Adding and subtracting $J_h'(\bar{U})$ gives

$$
\frac{\lambda}{4} \| \bar{U} - \bar{u} \|^2_{L^2(0,1)} \leq \langle J'(\bar{U}) - J_h'(\bar{U}), \bar{U} - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} + \langle J_h'(\bar{U}), \bar{U} - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} + \langle J'(\bar{u}), \bar{u} - \bar{U} \rangle_{L^2(0,1) \times L^2(0,1)}.
$$

Since $\langle J'(\bar{u}), \bar{u} - \bar{U} \rangle_{L^2(0,1) \times L^2(0,1)} \leq 0$, according to (2.8), we deduce

$$
\frac{\lambda}{4} \| \bar{U} - \bar{u} \|^2_{L^2(0,1)} \leq \langle J'(\bar{U}) - J_h'(\bar{U}), \bar{U} - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} + \langle J_h'(\bar{U}), \bar{U} - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)}.
$$

Add and subtract $\mathcal{P}_h \bar{u}$, the $L^2$ orthogonal projection of $\bar{u}$ onto $\mathbb{U}_{ad}$, to get

$$
\frac{\lambda}{4} \| \bar{U} - \bar{u} \|^2_{L^2(0,1)} \leq \langle J'(\bar{U}) - J_h'(\bar{U}), \bar{U} - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} + \langle J_h'(\bar{U}), \mathcal{P}_h \bar{u} - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} + \langle J_h'(\bar{U}), \bar{U} - \mathcal{P}_h \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)},
$$

Since $J_h'(\bar{U}) \in \mathbb{S}_h$ the middle term vanishes. In view of (4.6) and the fact that $\mathcal{P}_h \bar{u} \in \mathbb{U}_{ad}$, we deduce $\langle J_h'(\bar{U}), \bar{U} - \mathcal{P}_h \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)} \leq 0$ and

$$
\frac{\lambda}{4} \| \bar{U} - \bar{u} \|^2_{L^2(0,1)} \leq \langle J'(\bar{U}) - J_h'(\bar{U}), \bar{U} - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)},
$$

The explicit expressions $J'(\bar{U}) = \lambda \bar{U} + s(\bar{U})$ and $J_h'(\bar{U}) = \lambda \bar{U} + S(\bar{U})$ yield

$$
\frac{\lambda}{4} \| \bar{U} - \bar{u} \|^2_{L^2(0,1)} \leq \langle s(\bar{U}) - S(\bar{U}), \bar{U} - \bar{u} \rangle_{L^2(0,1) \times L^2(0,1)},
$$

which imply the desired estimate (6.1). □

**Corollary 6.2** (rate of convergence). *Let both $h_0$ and $\|v\|_{W^1_0(\Omega)}$ be sufficiently small. Furthermore, let $(s(\bar{U}), r(\bar{U}))$ be the solutions of the continuous adjoint equation (2.10) with $(\gamma(\bar{U}), y(\bar{U}))$ solutions for the continuous state equation (2.5b) with control $\bar{U}$. Let $(S(\bar{U}), R(\bar{U}))$ solve the discrete adjoint equation (4.5) with $(G(\bar{U}), Y(\bar{U}))$ solutions for the discrete state equation (4.4b) with control $\bar{U}$. If $h \leq h_0$, then there is a constant $C_0 \geq 1$, depending on $\|\gamma\|_{W^1_0(\Omega)}$, $\|y\|_{W^1_0(\Omega)}$, $\|s\|_{W^1_0(\Omega)}$, $\|r\|_{W^1_0(\Omega)}$, $\|\gamma_d\|_{L^2(\Omega)}$, $\|y_d\|_{L^2(\Omega)}$, such that

$$
\|\gamma(\bar{U}) - G(\bar{U})\|_{W^1_0(\Omega)} + \|y(\bar{U}) - Y(\bar{U})\|_{W^1_0(\Omega)} + \|s(\bar{U}) - S(\bar{U})\|_{W^1_0(\Omega)} + \|r(\bar{U}) - R(\bar{U})\|_{W^1_0(\Omega)} + \lambda \|\bar{U} - \bar{U}\|_{L^2(0,1)} \leq C_0 h. \tag{6.2}
$$

**Proof.** We combine the estimate

$$
\|s(\bar{U}) - S(\bar{U})\|_{L^2(0,1)} \leq \|s(\bar{U}) - S(\bar{U})\|_{W^1_0(\Omega)};
$$

with Lemma 5.6 for $u = \bar{U} = \bar{U}$

$$
\|s(\bar{U}) - S(\bar{U})\|_{L^2(0,1)} \leq C_1 h
$$
Our goal is to compute an approximation to the optimization problem presented in (6.2) set \( u = \bar{U} \), and \( U = \bar{U} \) in Lemmas 5.2, 5.3, 5.5 and 5.6 to complete the proof. \( \square \)

Remark 6.3 (linear rate). The first-order convergence rate of (6.2) is optimal for a piecewise-linear finite element discretization of \( (\gamma, y, s, r) \). For a control \( u \) in \( L^2 \), one might expect an increased rate of convergence. For example, it would be possible to use the standard Aubin-Nitsche duality argument if we were in a traditional linear setting to obtain

\[
\| s(\bar{U}) - S(\bar{U}) \|_{L^2(0,1)} \leq h^{1/2}\| s(\bar{U}) - S(\bar{U}) \|_{W^{1}_s(0,1)},
\]

which in turn would yield an optimal rate of convergence \( h^{3/2} \) for \( \bar{u} - \bar{U} \) in the proof of Corollary 6.2. Unfortunately, the duality method fails in our setting because the right-hand-side of the adjoint equations is discretized as well. Thus we are left merely with the Sobolev embedding

\[
\| s(\bar{U}) - S(\bar{U}) \|_{L^2(0,1)} \lesssim \| s(\bar{U}) - S(\bar{U}) \|_{W^{1}_s(0,1)}.
\]

In turn, this yields the linear rate of convergence for \( \bar{u} - \bar{U} \).

Remark 6.4 (dependence on \( k \)). Since \( k \) is the ellipticity constant for \( s \), then the estimate of \( u \) is inversely proportional to the surface tension coefficient \( k \) in view of (6.1).

7. Simulations. In our computations we assume the cost functional \( J \) in (2.5a) to be independent of \( y \) and \( y_\alpha \); we thus have

\[
J(\gamma, y, u) := \frac{1}{2}\| \gamma - \gamma_d \|_{L^2(0,1)}^2 + \frac{\lambda}{2}\| u \|_{L^2(0,1)}^2. \tag{7.1}
\]

Our goal is to compute an approximation to the optimization problem presented in (2.5) with the cost functional in (7.1). The Dirichlet data \( v = x_2(1 - x_2)(1 - 2x_1) \) applied to the entire boundary of \( \Omega \), and the desired configuration \( \gamma_d \) set to be an inverted hat function (see Figure 7.1). Moreover, we recall that \( \gamma \) satisfies the state equations (1.2b), and the second-order regularity \( \gamma \in W^{2}_\infty(0,1) \) (see Theorem 3.4), whence the profile \( \gamma_d \) is not achievable. We also remark that the curvature is not linearized as was done for the analysis of (2.5b) and (2.1).

In view of the control constraint \( u \in \mathcal{U}_\text{ad} \) (2.6), we need \( \| u \|_{L^2(0,1)} \leq \theta_1/2\alpha \). Since \( \alpha \sim 1/k \) and \( \theta_1 < 1 \), we have \( \| u \|_{L^2(0,1)} \sim \kappa \). In our computations we have \( \kappa \leq 1 \), this motivates us to consider the following set for the admissible controls.

\[
\mathcal{U}_\text{ad} = \left\{ u \in L^2(0,1) : \| u \|_{L^2(0,1)} \leq 3 \right\}.
\]

We discretize the state variables \( (\gamma, y) \), the adjoint variables \( (s, r) \) and the control \( u \) using piecewise bi-linear finite elements. We remark that in our case the first optimize then discretize approach is equivalent to first discretize then optimize (see [9] p. 160-164)]. To solve the state equations we use an affine invariant Newton strategy from [9] NLEQ-ERR, p. 148-149] because of its local quadratic convergence. The weak adjoint equations (2.10), or (3.15) in strong form, involve the coupling between the 2d bulk and 1d interface. This seemingly complicated coupling might entail an unusual assembly procedure and geometric mesh restrictions to evaluate integrals in (2.12). This is fortunately not the case because the matrix of the adjoint
system happens to be the transpose of the Jacobian of the state equations, according to Lemma 2.1, which is available to us from the Newton method. The assembly can thus be done with ease. We work on the platform provided by the deal.II finite element library and use a direct (built-in) solver to invert the Jacobian at every Newton iteration, as well as the linear adjoint algebraic system. Consequently we can compute the derivative \( J' \) of the cost functional.

We use a gradient based minimization algorithm to solve the minimization problem in Matlab. In particular, we use the built-in Matlab functions \texttt{fmincon} (constrained case), and \texttt{fminunc} (unconstrained case). Stopping criterion: the optimization algorithm stops when the gradient of the cost function is less than or equal to \( \lambda \cdot 1e^{-4} \), or if the difference between two consecutive values of the cost function are less than or equal to \( \lambda \cdot 1e^{-4} \).

We present two examples to illustrate our theoretical a priori estimate for the control in Corollary 6.2. In particular, we study the behavior of the solution as the regularization parameter \( \lambda \) goes to zero; they differ on whether or not the control is a constrained quantity.

For each of these examples we collect the following metrics

- The cost function value \( J(\bar{u}) \).
- The smallest eigenvalue of \( J''(\bar{u}) \), representing the constant \( \delta \) in the 2nd order sufficient condition \( J''(\bar{u}) h^2 \geq \delta \| h \|^2_{L^2(0,1)} \). This metric is obtained in Matlab through the approximated Hessian provided by the \texttt{fmincon} or \texttt{fminunc} functions.
- The discrete \( L^2 \) norm of the optimal control \( \bar{u} \) is equal to \( (\bar{u}^T M \bar{u})^{1/2} \), where \( M \) denotes the mass matrix corresponding to 1d problem in the interval \((0,1)\).
- The “self-convergence” rate of the optimal control as we uniformly refine the finite element mesh. We first solve the problem on a very fine mesh, 8 uniform refinement cycles, and use it in place of a closed form solution. Deriving a closed form solution to a nonlinear optimization problem is rather complicated and thus impractical.

| \( \lambda \) | 1   | 1e-1 | 1e-2 | 1e-3 | 1e-4 | 1e-5 | 1e-6 |
|----------------|-----|------|------|------|------|------|------|
| \( J(\bar{u}) \) | 7.32e-2 | 6.27e-2 | 2.77e-2 | 7.80e-3 | 1.60e-3 | 2.52e-4 | 4.20e-5 |
| \( J''(\bar{u}) \) | 7.56e-2 | 8.10e-3 | 1.30e-3 | 6.24e-4 | 5.57e-4 | 5.50e-4 | 5.49e-4 |
| \( \| \bar{u} \|_{L^2(\Gamma)} \) | 0.05 | 0.45 | 1.71 | 3.00 | 5.00 | 6.30 | 8.06 |
| rate            | 1.1610 | 2.0202 | 1.1224 | 1.8402 | 1.70 | 1.5019 | 1.2117 |

\textbf{Table 7.1}

Example 1 (Unconstrained case): the values of the cost function \( J(\bar{u}) \), the smallest eigenvalue of \( J''(\bar{u}) \), the \( L^2 \)-norm of \( \bar{u} \) and the convergence rate of optimal control as \( \lambda \) varies from 1 to 1e-6.
7.1. Example 1: Unconstrained control. We begin with the nominal case 
\( u \in L^2(0,1) \) and \( \kappa = 1 \), i.e. the control is unconstrained and the surface tension coefficient is fixed. We are interested in the metrics \( J(\bar{u}), J''(\bar{u}), \|\bar{u}\|_{L^2(\Gamma)} \) and convergence rate as the control regularization parameter \( \lambda \) approaches zero; see Table 7.1.

Recall that we used a fixed point argument to prove the existence and uniqueness of a solution for the state equations which required \( \bar{u} \in \mathcal{U}_{ad} \). For \( \lambda = 1e-6 \), we have \( \|\bar{u}\|_{L^2(0,1)} = 8 \), i.e. \( \bar{u} \notin \mathcal{U}_{ad} \). Nevertheless, we can still solve the state equations. This indicates that our choice of \( \mathcal{U}_{ad} \) is not sharp and we can solve the state equations even for larger \( \bar{u} \).

The smallest eigenvalue of the approximated Hessian \( J''(\bar{u}) \) for \( \lambda = 1e-6 \) is \( 5e^{-4} \) i.e. the control \( \bar{u} \) is also locally unique. The last row in Table 7.1 justifies the theoretical findings in Corollary 6.2.

| \( (\gamma, y) \) | \( \bar{u} \) | \( (\gamma, y) \) | \( \bar{u} \) |
|---|---|---|---|
| \( \lambda = \infty, \bar{u} \in [0,0] \) | | \( \lambda = 1e-3, \bar{u} \in (-5.38,0.93) \) |
| \( \lambda = 1, \bar{u} \in (-0.0784971,0] \) | | \( \lambda = 1e-4, \bar{u} \in (-9.78,4.96) \) |
| \( \lambda = 1e-1, \bar{u} \in (-0.675277,0] \) | | \( \lambda = 1e-5, \bar{u} \in (-17.63,6.07) \) |
| \( \lambda = 1e-2, \bar{u} \in (-2.65675,0] \) | | \( \lambda = 1e-6, \bar{u} \in (-33.1146,6.73) \) |

Fig. 7.2. Example 1 (Unconstrained case): The optimal state solution \( (\gamma, y) \), the applied control \( \bar{u} \) in solid blue, and the previous control in dashed red for comparison. Each picture displays the corresponding value of \( \lambda \) from \( \lambda = \infty \) to \( \lambda = 1e-6 \).

The first column in Figure 7.2 shows the optimal state \( (\gamma, y) \) as \( \lambda \) approaches zero. The second column shows the control applied (solid blue); for reference we also
plot the previous control (dotted red). For \( \lambda = 1 \) to \( \lambda = 1e-2 \) one can see that the control acts at the center and tries to move \( \gamma \) towards \( \gamma_d \). For \( \lambda = 1e-3 \) the control needs to push \( \gamma \) in the right-half up, and in the left-half down and therefore it adjusts accordingly. For \( \lambda = 1e-6 \) the control again mostly acts at the center. Moreover \( \gamma \) matches \( \gamma_d \) almost perfectly.

### 7.2. Example 2: Constrained Control

This example differs from Example 1 only due to the fact that now we impose \( u \in U_{ad} \). The metrics are shown in Table 7.2.

We first remark that, as in the previous example, the control is locally unique and the control convergence rate is linear.

| \( \lambda \) | \( \infty \) | 1 | 1e-1 | 1e-2 | 1e-3 | 1e-4 | 1e-5 |
|---|---|---|---|---|---|---|---|
| \( \mathcal{J}(\bar{u}) \) | 0.07462 | 0.07317 | 0.06276 | 0.02773 | 0.00780 | 0.00375 | 0.00334 |
| \( \mathcal{J}''(\bar{u}) \) | - | 0.8571 | 0.5143 | 0.8571 | 0.1429 | 8.49e-5 | 9.74e-5 |
| \( \|\bar{u}\|_{L^2(\Gamma)} \) | 0 | 0.0516 | 0.4415 | 1.7092 | 2.9970 | 3 | 3 |
| rate | - | 1.4353 | 2.7840 | 1.2716 | 1.5117 | 1.2134 | 1.1942 |

**Table 7.2**

Constrained case: the values of the cost function \( \mathcal{J}(\bar{u}) \), the smallest eigenvalue of \( \mathcal{J}''(\bar{u}) \), the \( L^2 \)-norm of \( \bar{u} \) and the convergence rate of the optimal control as \( \lambda \) approaches 0. Notice that the constraint is active for \( \lambda = 1e-4 \) and \( 1e-5 \).

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**Fig. 7.3. Example 2 (Constrained case):** The optimal state solution \( (\bar{\gamma}, \bar{y}) \), the applied control \( \bar{u} \) in solid blue, and the previous control in dashed red for comparison. The pictures show the corresponding value of \( \lambda \), from \( \lambda = 1 \) to \( \lambda = 1e-5 \), as well as the smallest and largest value of control. Notice that there is no visual difference between the optimal control for \( \lambda = 1e-3, 1e-4 \) and \( 1e-5 \). This is because the control constraints are active.
When $\lambda = 1e-4$ the control constraints become active and as a result the reduction in the cost function is severely impacted. This becomes clear after comparing the constrained and unconstrained cases for $\lambda = 1e-5$.

Figure 7.3 shows the optimal state $(\bar{\gamma}, \bar{y})$ and the two consecutive optimal controls (blue: current, red: previous). For $\lambda = 1e-4$ and $1e-5$ the current and previous controls lie on top of each other because the constraints are active. We also remark that we can not get as close to the desired configuration $\gamma_d$ as in the unconstrained case due to the constraint.

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REFERENCES

[1] H. Antil, R. H. Nochetto, and P. Sodré, Optimal control of a free boundary problem: Analysis with second order sufficient conditions, Submitted. arXiv preprint arXiv:1210.0031, (2012).
[2] N. Arada, E. Casas, and F. Tröltzsch, Error estimates for the numerical approximation of a semilinear elliptic control problem, Comput. Optim. Appl., 23 (2002), pp. 201–229.
[3] W. Bangerth, R. Hartmann, and G. Kanschat, deal.II – a general purpose object oriented finite element library, ACM Trans. Math. Softw., 33 (2007), pp. 24/1–24/27.
[4] S. C. Brenner and L. R. Scott, The Mathematical Theory of Finite Element Methods, vol. 15 of Texts in Applied Mathematics, Springer, New York, third ed., 2008.
[5] E. Casas, M. Mateos, and F. Tröltzsch, Error estimates for the numerical approximation of boundary semilinear elliptic control problems, Comput. Optim. Appl., 31 (2005), pp. 193–219.
[6] P. Deuflhard, Newton Methods for Nonlinear Problems - Affine Invariance and Adaptive Algorithms, vol. 35 of Springer Series in Computational Mathematics, Springer-Verlag, Berlin, 2004.
[7] D. Gilbarg and N. S. Trudinger, Elliptic Partial Differential Equations of Second Order, Classics in Mathematics, Springer-Verlag, Berlin, 2001. Reprint of the 1998 edition.
[8] M. Hinze, A variational discretization concept in control constrained optimization: the linear-quadratic case, Comput. Optim. Appl., 30 (2005), pp. 45–61.
[9] M. Hinze, R. Pinnau, M. Ulbrich, and S. Ulbrich, Optimization with PDE constraints, vol. 23 of Mathematical Modelling: Theory and Applications, Springer, New York, 2009.
[10] A. Rösch, Error estimates for linear-quadratic control problems with control constraints, Optim. Methods Softw., 21 (2006), pp. 121–134.
[11] P. Saavedra and L. R. Scott, Variational formulation of a model free-boundary problem, Math. Comp., 57 (1991), pp. 451–475.
[12] V. A. Solonnikov, On the stokes equations in domains with non-smooth boundaries and on viscous incompressible flow with a free surface, in Nonlinear partial differential equations and their applications: Collège de France seminar, vol. 3, Pitman Publishing (UK), 1982, pp. 340–423.