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AN IMPROVED ERROR ANALYSIS FOR FINITE ELEMENT APPROXIMATION OF BIOLUMINESCENCE TOMOGRAPHY*

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Dedicated to Professor Junzhi Cui on the occasion of his 70th birthday

Abstract

This paper is concerned with an ill-posed problem which results from the area of molecular imaging and is known as BLT problem. Using Tikhonov regularization technique, a quadratic optimization problem can be formulated. We provide an improved error estimate for the finite element approximation of the regularized optimization problem. Some numerical examples are presented to demonstrate our theoretical results.

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1. Introduction

In modern medical science, molecular imaging plays an important role. The traditional imaging techniques such as computed tomography (CT), magnetic resonance imaging (MRI) [12] can not fulfill the requirements, so optical imaging methods such as florescence molecular tomography (FMT) [13] and bioluminescence imaging (BLT) [14] are becoming flourishing in the decades. Bioluminescence imaging is based on the use of a family of enzymes known as luciferases, which are found in organisms that emit a bioluminescent glow. It can be applied to all disease processes in all areas of small-animal models. Examples of ongoing applications include cancer, inflammatory disease, neurodegenerative disease, gastrointestinal physiology, renal physiology, cell trafficking, stem cell research, transplant science, and muscle physiology.

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The bioluminescent photon transport in the media can be described by radiative transfer equation, which can be reduced to a diffusion equation [12]:

$$-\text{div}(D\nabla y) + \mu y = u \quad \text{in} \ \ \Omega, \tag{1.1}$$

$$y + 2(D\nabla y)\cdot n = g^- \quad \text{on} \ \ \partial\Omega. \tag{1.2}$$

We should find a source function u in view of the boundary value problems (1.1)-(1.2) and accordant with the measurement g on the boundary by $(D\nabla y)\cdot n = -g$. This is a typical inverse source problem and is proved strongly ill-posed. Through a Tikhonov regularization technique, a well-posed optimization problem to approximate the original BLT problem is proposed in [5], both convergence analysis and numerical treatment are provided.

In this paper, we analyze the regularized optimization scheme proposed in [5] using the analysis technique for optimal control problems. By introducing an adjoint state, the optimization problem can be converted to a system with three coupled equations. Then the analysis for both the continuous and discretized systems are clearer and easier. Using the a new methodology in the a priori error analysis for the finite element approximation of the regularized optimization problem, an improved error estimate is obtained comparing to the results in [5]. Numerical experiments confirm our results.

The paper is organized as follows: In Section 2, we introduce the mathematical model of bioluminescence tomography. In Section 3, the finite element scheme of the model problem is presented. Then the improved a priori error analysis is provided in Section 4. In the last section, some numerical results on the model problem are provided.

2. The Mathematical Model of Bioluminescence Tomography

Let us consider the following ill-posed problem:

$$-\text{div}(D\nabla y) + \mu y = Bu \quad \text{in} \ \ \Omega, \tag{2.1}$$

$$y + 2(D\nabla y)\cdot n = g^- \quad \text{on} \ \ \partial\Omega, \tag{2.2}$$

$$(D\nabla y)\cdot n = -g \quad \text{on} \ \partial\Omega, \tag{2.3}$$

where Ω is a bounded domain in $\mathbb{R}^n (n \leq 3)$ with a Lipschitz boundary $\Gamma = \partial\Omega$, D is a symmetric or nonsymmetric positive definite matrix, $\mu \geq 0$, n is the outward normal on $\partial\Omega$, B is a linear operator from Ω_U to Ω, which has the typical form of a characteristic function χ_{Ω_U} on $\Omega_U \subset \Omega$.

In above problem, g^- is usually a given function and is zero in a typical BLT problem, whereas g is the measurement. We should detect the source function u by the measurement g, and u is usually in a closed convex subset Q_U of the space $L^2(\Omega_U)$. In the typical BLT problems Q_U has usually the form of $L^2(\Omega_U)$ or the subset of $L^2(\Omega_U)$ with nonnegatively valued functions. From the boundary conditions (2.2) and (2.3) we can formulate another boundary condition:

$$y = g^- + 2g \quad \text{on} \ \ \Gamma.$$

Then we will only consider the following two boundary conditions to fix the idea

$$y = g_1 \quad \text{on} \ \ \Gamma, \tag{2.4}$$

$$(D\nabla y)\cdot n = g_2 \quad \text{on} \ \ \Gamma. \tag{2.5}$$

It is well known that the problem (2.1) with boundary conditions (2.4) and (2.5) has infinitely many solutions. Using Tikhonov regularization strategy, a regularized optimization problem is provided in [5] as

$$\min_{u_\epsilon \in Q_U} \left\{ \frac{1}{2}\|y_\epsilon - g_1\|^2_{L^2(\Gamma)} + \frac{\epsilon}{2}\|u_\epsilon\|^2_{L^2(\Omega_U)} \right\} \tag{2.6}$$

subject to

$$-\text{div}(D\nabla y_\epsilon) + \mu y_\epsilon = Bu_\epsilon \quad \text{in} \ \ \Omega, \tag{2.7}$$

$$(D\nabla y_\epsilon)\cdot n = g_2 \quad \text{on} \ \ \Gamma. \tag{2.8}$$

By the Lax-Milgram Lemma, it is well known that problem (2.7)-(2.8) has a unique solution $y_\epsilon(u_\epsilon)$ for all $u_\epsilon \in L^2(\Omega_U)$. Let

$$J_\epsilon(u_\epsilon) = \frac{1}{2}\|y_\epsilon - g_1\|^2_{L^2(\Gamma)} + \frac{\epsilon}{2}\|u_\epsilon\|^2_{L^2(\Omega_U)}.$$

It is clearly that the quadratic functional J_ϵ is strictly convex, so that the minimization problem (2.6)-(2.8) admits a unique solution. Furthermore, it has been proved in [5] that the regularized optimization problem is stable and the solution of problem (2.6) u_ϵ converges to the solution of BLT problem strongly in the sense of L^2-norm when $\epsilon \to 0$.

Let

$$\begin{aligned}
&a(y,v) = \int_\Omega (D\nabla y\nabla v + \mu yv)dx, \ \forall \ y, \ v\in H^1(\Omega),\\
&(u,v) = \int_\Omega uvdx, \ \forall \ u, \ v\in L^2(\Omega),\\
&(u,v)_U = \int_{\Omega_U} uvdx, \ \forall \ u, \ v\in L^2(\Omega_U),\\
&< y,v >= \int_\Gamma yvds, \ \forall \ y, \ v\in L^2(\Gamma).
\end{aligned}$$

Then following the lines of [9] we have that the pair (y_ϵ, u_ϵ) is the solution of the problem (2.6)-(2.8) if and only if there exists an adjoint state $p_\epsilon \in H^1(\Omega)$ such that

$$a(y_\epsilon, v) = (Bu_\epsilon, v) + < g_2, v >, \ \forall \ v \in H^1(\Omega), \tag{2.9}$$

$$a(w, p_\epsilon) =< y_\epsilon - g_1, w >, \ \forall \ w\in H^1(\Omega), \tag{2.10}$$

$$(B^* p_\epsilon + \epsilon u_\epsilon, v - u_\epsilon)_U \geq 0, \ \forall \ v\in Q_U, \tag{2.11}$$

where B^* is the adjoint of B.

3. The Finite Element Approximation

In this section, we consider the finite element approximation of the regularized optimization problem (2.6)-(2.8).

Let Ω^h be a polygonal approximation to Ω with a boundary $\partial\Omega^h$. For simplicity, we assume that $\Omega^h = \Omega$. Let $\mathcal{T}^h$ be a partitioning of Ω^h into disjoint regular $n-$simplices τ such that $\bar{\Omega}^h = \bigcup_{\tau\in\mathcal{T}^h} \bar{\tau}$. Associated with $\mathcal{T}^h$ is a finite dimensional subspace V^h of $C(\bar{\Omega}^h)$, such that

$v|_\tau$ are polynomials of m-order($m \geq 1$) $\forall\ v \in V^h$ and $\tau \in \mathcal{T}^h$. In this paper, we only consider the case $m = 1$ for V^h.

Let $\mathcal{T}_U^h$ be a partitioning of Ω_U^h into disjoint regular $n-$simplices τ_U such that $\bar{\Omega}_U^h = \bigcup_{\tau_U \in \mathcal{T}_U^h} \bar{\tau}_U$. Again, assume that $\Omega_U^h = \Omega_U$. Associated with $\mathcal{T}_U^h$ is another finite dimensional subspace W_U^h of $L^2(\Omega_U^h)$, such that $w|_{\tau_U}$ are polynomials of $l-$order($l \geq 0$) $\forall w \in W_U^h$ and $\tau_U \in \mathcal{T}_U^h$. Let $Q_U^h = Q_U \cap W_U^h$. In this paper, we consider the cases $l = 0$ or $l = 1$ for W_U^h.

In the following, we will denote h_τ and h_{τ_U} the diameters of the element $\tau \in \mathcal{T}^h$ and $\tau_U \in \mathcal{T}_U^h$, respectively. Set $h = \max_{\tau \in \mathcal{T}^h} h_\tau$ and $h_U = \max_{\tau_U \in \mathcal{T}_U^h} h_{\tau_U}$.

Then the finite element approximation of the problem (2.6) reads as

$$\min_{u_\epsilon^h \in Q_U^h} \left\{ \frac{1}{2} \|y_\epsilon^h - g_1\|^2_{L^2(\Gamma)} + \frac{\epsilon}{2} \|u_\epsilon^h\|^2_{L^2(\Omega_U)} \right\}, \tag{3.1}$$

subject to

$$a(y_\epsilon^h, v^h) = (Bu_\epsilon^h, v^h) + < g_2, v^h > \quad \forall\ v^h \in V^h.$$

Again, it follows that the problem (3.1) has a solution $(y_\epsilon^h, u_\epsilon^h)$, and a pair $(y_\epsilon^h, u_\epsilon^h) \in V^h \times Q_U^h$ is the solution of (3.1) if and only if there is a co-state $p_\epsilon^h \in V^h$ such that the triplet $(y_\epsilon^h, p_\epsilon^h, u_\epsilon^h)$ satisfies the following optimality conditions:

$$a(y_\epsilon^h, v^h) = (Bu_\epsilon^h, v^h) + < g_2, v^h >,\ \forall\ v^h \in V^h, \tag{3.2}$$

$$a(w^h, p_\epsilon^h) = < y_\epsilon^h - g_1, w^h >,\ \forall\ w^h \in V^h, \tag{3.3}$$

$$(B^* p_\epsilon^h + \epsilon u_\epsilon^h, v^h - u_\epsilon^h)_U \geq 0,\ \forall\ v^h \in Q_U^h. \tag{3.4}$$

The theoretical analysis concludes that the solution of above finite element scheme (3.2)-(3.4) approximates the solution of the regularized optimization problem (2.6)-(2.8) (see [5] and the next section). Moreover, it has been shown in [5] that the solution of (2.6)-(2.8) approximates the exact solution of the original problem (2.1) with the boundary conditions (2.4) and (2.5), when ϵ goes to zero. Then it is clear that we can use the finite element scheme presented in this section to make the numerical simulation for the BLT problem.

4. Error Analysis

In this section, we will discuss the error analysis of the finite element approximation provided in the last section. As mentioned in Section 2, we will only consider the two types of control set: $Q_U = L^2(\Omega_U)$ or $Q_U = \{v \in L^2(\Omega_U),\ v \geq 0 \text{ a.e. in } \Omega_U\}$. At first, we consider the case $l = 0$, i.e., we approximate the control by piecewise constant finite element space. The finite element space for the state and the costate is conforming piecewise linear ($m = 1$).

Theorem 4.1. *Let* $(y_\epsilon, p_\epsilon, u_\epsilon)$ *be the solution of problem* (2.9)-(2.11), $(y_\epsilon^h, p_\epsilon^h, u_\epsilon^h)$ *be the solution of problem* (3.2)-(3.4). *Assume that* Ω *is convex,* $D \in (C(\Omega))_{2\times 2}$, $u_\epsilon \in H^1(\Omega_U)$, $y_\epsilon, p_\epsilon \in H^2(\Omega)$. *Then we have*

$$\epsilon \|u_\epsilon - u_\epsilon^h\|^2_{0,\Omega_U} + \|y_\epsilon - y_\epsilon^h\|^2_{0,\Gamma} + \|p_\epsilon - p_\epsilon^h\|^2_{1,\Omega} \leq Ch^2 + Ch_U^2. \tag{4.1}$$

Proof. Let $(y_\epsilon^h(u_\epsilon), p_\epsilon^h(u_\epsilon)) \in V^h \times V^h$ be the solution of the following auxiliary problem:

$$a(y_\epsilon^h(u_\epsilon), v_h) = (Bu_\epsilon, v_h) + < g_2, v_h >,\ \forall v_h \in V^h, \tag{4.2}$$

$$a(w_h, p_\epsilon^h(u_\epsilon)) = < y_\epsilon^h(u_\epsilon) - g_1, w_h >,\ \forall w_h \in V^h. \tag{4.3}$$

Then we have

$$\begin{aligned}(B^*p_\epsilon^h(u_\epsilon)-B^*p_\epsilon^h,u_\epsilon-u_\epsilon^h)_U &= (p_\epsilon^h(u_\epsilon)-p_\epsilon^h,B(u_\epsilon-u_\epsilon^h))\\ &= a(y_\epsilon^h(u_\epsilon)-y_\epsilon^h,p_\epsilon^h(u_\epsilon)-p_\epsilon^h)\\ &= < y_\epsilon^h(u_\epsilon)-y_\epsilon^h,y_\epsilon^h(u_\epsilon)-y_\epsilon^h >\\ &= \|y_\epsilon^h(u_\epsilon)-y_\epsilon^h\|_{0,\Gamma}^2. \end{aligned} \tag{4.4}$$

Let u^I be the integral average of u on the element such that

$$u^I|_{\tau_U}=\frac{\int_{\tau_U}u}{\int_{\tau_U}1}.$$

Then $u^I\in Q_U^h$, and it is well known (see, e.g., [2]) that for all $w\in H^1(\Omega_U)$,

$$\|w-w^I\|_{0,\Omega_U}\le Ch_U\|w\|_{1,\Omega_U}. \tag{4.5}$$

Note that $u_\epsilon\in H^1(\Omega_U)$, $u_\epsilon^h\in L^2(\Omega_U)$, and $p_\epsilon^h\in H^1(\Omega)$. It follows from (2.11), (3.4) and (4.4)-(4.5) that

$$\begin{aligned}&\epsilon\|u_\epsilon-u_\epsilon^h\|_{0,\Omega_U}^2+\|y_\epsilon^h-y_\epsilon^h(u_\epsilon)\|_{0,\Gamma}^2\\ =\ &(B^*p_\epsilon^h(u_\epsilon)+\epsilon u_\epsilon,u_\epsilon-u_\epsilon^h)_U-(B^*p_\epsilon^h+\epsilon u_\epsilon^h,u_\epsilon-u_\epsilon^h)_U\\ =\ &(B^*p_\epsilon+\epsilon u_\epsilon,u_\epsilon-u_\epsilon^h)_U+(B^*p_\epsilon^h(u_\epsilon)-B^*p_\epsilon,u_\epsilon-u_\epsilon^h)_U\\ &+(B^*p_\epsilon^h+\epsilon u_\epsilon^h,u_\epsilon^h-u_\epsilon^I)_U+(B^*p_\epsilon^h+\epsilon u_\epsilon^h,u_\epsilon^I-u_\epsilon)_U\\ \le\ &0+\|B^*(p_\epsilon^h(u_\epsilon)-p_\epsilon)\|_{0,\Omega_U}\|u_\epsilon-u_\epsilon^h\|_{0,\Omega_U}+0+(B^*p_\epsilon^h,u_\epsilon^I-u_\epsilon)_U\\ \le\ &C\|p_\epsilon^h(u_\epsilon)-p_\epsilon\|_{0,\Omega}+(B^*p_\epsilon^h-(B^*p_\epsilon^h)^I,u_\epsilon^I-u_\epsilon)_U.\\ \le\ &C\|p_\epsilon^h(u_\epsilon)-p_\epsilon\|_{0,\Omega}+Ch_U^2\|B^*p_\epsilon^h\|_{1,\Omega_U}\|u_\epsilon\|_{1,\Omega_U}. \end{aligned} \tag{4.6}$$

Next, let us consider the error $\|p_\epsilon^h(u_\epsilon)-p_\epsilon\|_{0,\Omega}$. Let $\pi_h: C(\Omega)\to V^h$ be the standard piecewise linear Lagrange interpolation operator. Note that the bilinear form $a(\cdot,\cdot)$ is positive definite and $\|w\|_{\frac12,\partial\Omega}\le C\|w\|_{1,\Omega}$. It can be derived from (2.10) and (4.3) that

$$\begin{aligned}&c\|p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon\|_{1,\Omega}^2\\ \le\ &a(p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon,p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon)\\ =\ &a(p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon,p_\epsilon^h(u_\epsilon)-p_\epsilon)+a(p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon,p_\epsilon-\pi_hp_\epsilon)\\ =\ &< y_\epsilon^h(u_\epsilon)-y_\epsilon,p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon > +a(p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon,p_\epsilon-\pi_hp_\epsilon)\\ \le\ &C(\|y_\epsilon^h(u_\epsilon)-y_\epsilon\|_{-\frac12,\Gamma}+\|p_\epsilon-\pi_hp_\epsilon\|_{1,\Omega})\|p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon\|_{1,\Omega}, \end{aligned}$$

which implies that

$$\|p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon\|_{1,\Omega}\le C\|y_\epsilon^h(u_\epsilon)-y_\epsilon\|_{-\frac12,\Gamma}+C\|p_\epsilon-\pi_hp_\epsilon\|_{1,\Omega},$$

and

$$\begin{aligned}\|p_\epsilon^h(u_\epsilon)-p_\epsilon\|_{1,\Omega} &\le \|p_\epsilon^h(u_\epsilon)-\pi_hp_\epsilon\|_{1,\Omega}+\|\pi_hp_\epsilon-p_\epsilon\|_{1,\Omega}\\ &\le C\|y_\epsilon^h(u_\epsilon)-y_\epsilon\|_{-\frac12,\Gamma}+C\|p_\epsilon-\pi_hp_\epsilon\|_{1,\Omega}\\ &\le C\|y_\epsilon^h(u_\epsilon)-y_\epsilon\|_{-\frac12,\Gamma}+Ch\|p_\epsilon\|_{2,\Omega}, \end{aligned} \tag{4.7}$$

where we used the well known interpolation error estimate: $\|w-\pi_h w\|_{1,\Omega} \le Ch\|w\|_{2,\Omega}$ for all $w \in H^2(\Omega)$ (see, e.g., [2]).

Then we consider the error $\|y_\epsilon^h(u_\epsilon) - y_\epsilon\|_{-\frac{1}{2},\Gamma}$. Noting that $y_\epsilon^h(u_\epsilon)$ is the standard finite element approximation of $y_\epsilon(u_\epsilon)$, from the finite element error analysis (see, e.g., [2]) we have

$$\|y_\epsilon^h(u_\epsilon) - y_\epsilon\|_{1,\Omega} \le Ch\|y_\epsilon\|_{2,\Omega}. \tag{4.8}$$

For all $g \in H^{\frac{1}{2}}(\Gamma)$, set ψ be the solution of the following equation:

$$\begin{aligned} &-\mathrm{div}(D^*\nabla\psi) + \mu\psi = 0 \quad \text{in } \ \Omega, \\ &(D^*\nabla\psi)\cdot n = g \quad \text{on } \ \Gamma, \end{aligned}$$

where D^* is the conjugate matrix of D. Noting that Ω is convex and $D \in (C(\Omega))_{2\times 2}$, we have $\|\psi\|_{2,\Omega} \le C\|g\|_{\frac{1}{2},\Gamma}$. Using the well known duality argument, we can obtain that

$$\begin{aligned} < y_\epsilon^h(u_\epsilon) - y_\epsilon, g > &= a(y_\epsilon^h(u_\epsilon) - y_\epsilon, \psi) = a(y_\epsilon^h(u_\epsilon) - y_\epsilon, \psi - \pi_h\psi) \\ &\le C\|y_\epsilon^h(u_\epsilon) - y_\epsilon\|_{1,\Omega}\|\psi - \pi_h\psi\|_{1,\Omega} \le Ch^2\|y_\epsilon\|_{2,\Omega}\|\psi\|_{2,\Omega} \\ &\le Ch^2\|y_\epsilon\|_{2,\Omega}\|g\|_{\frac{1}{2},\Gamma}. \end{aligned}$$

Therefore, we have that

$$\|y_\epsilon^h(u_\epsilon) - y_\epsilon\|_{-\frac{1}{2},\Gamma} = \sup_{g\in H^{\frac{1}{2}}(\Gamma)} \frac{< y_\epsilon^h(u_\epsilon) - y_\epsilon, g >}{\|g\|_{\frac{1}{2},\Gamma}} \le Ch^2\|y_\epsilon\|_{2,\Omega}. \tag{4.9}$$

Thus it is concluded from (4.7) and (4.9) that

$$\|p_\epsilon^h(u_\epsilon) - p_\epsilon\|_{1,\Omega} \le Ch^2\|y_\epsilon\|_{2,\Omega} + Ch\|p_\epsilon\|_{2,\Omega}. \tag{4.10}$$

Furthermore, for all $f \in L^2(\Omega)$, set φ be the solution of the following equation:

$$\begin{aligned} &-\mathrm{div}(D\nabla\varphi) + \mu\varphi = f, \quad \text{in } \ \Omega, \\ &(D\nabla\varphi)\cdot n = 0, \quad \text{on } \ \Gamma. \end{aligned}$$

Again noting that Ω is convex and $D \in (C(\Omega))_{2\times 2}$, we have

$$\|\varphi\|_{2,\Omega} \le C\|f\|_{0,\Omega}.$$

Then it follows from (4.9) and (4.10) that

$$\begin{aligned} &(p_\epsilon^h(u_\epsilon) - p_\epsilon, f) = a(\varphi, p_\epsilon^h(u_\epsilon) - p_\epsilon) \\ &= a(\varphi - \pi_h\varphi, p_\epsilon^h(u_\epsilon) - p_\epsilon) + a(\pi_h\varphi, p_\epsilon^h(u_\epsilon) - p_\epsilon) \\ &\le C\|p_\epsilon^h(u_\epsilon) - p_\epsilon\|_{1,\Omega}\|\varphi - \pi_h\varphi\|_{1,\Omega} + < y_\epsilon^h(u_\epsilon) - y_\epsilon, \pi_h\varphi > \\ &\le Ch\|p_\epsilon^h(u_\epsilon) - p_\epsilon\|_{1,\Omega}\|\varphi\|_{2,\Omega} + C\|y_\epsilon^h(u_\epsilon) - y_\epsilon\|_{-\frac{1}{2},\partial\Omega}\|\pi_h\varphi\|_{\frac{1}{2},\partial\Omega} \\ &\le Ch^2(\|p_\epsilon\|_{2,\Omega} + \|y_\epsilon\|_{2,\Omega})\|\varphi\|_{2,\Omega} \\ &\le Ch^2(\|p_\epsilon\|_{2,\Omega} + \|y_\epsilon\|_{2,\Omega})\|f\|_{0,\Omega}. \end{aligned} \tag{4.11}$$

Therefore by the definition of the norm we have

$$\begin{aligned} \|p_\epsilon^h(u_\epsilon) - p_\epsilon\|_{0,\Omega} &= \sup_{f\in L^2(\Omega)} \frac{(p_\epsilon^h(u_\epsilon) - p_\epsilon, f)}{\|f\|_{0,\Omega}} \\ &\le Ch^2(\|p_\epsilon\|_{2,\Omega} + \|y_\epsilon\|_{2,\Omega}). \end{aligned} \tag{4.12}$$

and then (4.6) and (4.12) imply that

$$\epsilon\|u_\epsilon - u_\epsilon^h\|_{0,\Omega_U}^2 + \|y_\epsilon^h - y_\epsilon^h(u_\epsilon)\|_{0,\Gamma}^2 \le C(h^2 + h_U^2). \tag{4.13}$$

Applying the error estimate (4.8) and the trace theorem:

$$\|v\|_{0,\Gamma} \le C\|v\|_{1,\Omega}, \ \forall v \in H^1(\Omega),$$

we have

$$\begin{aligned}\|y_\epsilon - y_\epsilon^h\|_{0,\Gamma}^2 &\le \|y_\epsilon - y_\epsilon^h(u_\epsilon)\|_{0,\Gamma}^2 + \|y_\epsilon^h(u_\epsilon) - y_\epsilon^h\|_{0,\Gamma}^2 \\ &\le C\|y_\epsilon - y_\epsilon^h(u_\epsilon)\|_{1,\Omega}^2 + C(h^2 + h_U^2) \\ &\le C(h^2 + h_U^2).\end{aligned} \tag{4.14}$$

On the other hand,

$$\begin{aligned}c\|p_\epsilon^h(u_\epsilon) - p_\epsilon^h\|_{1,\Omega}^2 &\le a(p_\epsilon^h(u_\epsilon) - p_\epsilon^h, p_\epsilon^h(u_\epsilon) - p_\epsilon^h) \\ &= < y_\epsilon^h(u_\epsilon) - y_\epsilon^h, p_\epsilon^h(u_\epsilon) - p_\epsilon^h > \\ &\le C\|y_\epsilon^h(u_\epsilon) - y_\epsilon^h\|_{0,\Gamma}\|p_\epsilon^h(u_\epsilon) - p_\epsilon^h\|_{1,\Omega}.\end{aligned} \tag{4.15}$$

Then from (4.10), (4.13) and (4.15) we have that

$$\begin{aligned}\|p_\epsilon - p_\epsilon^h\|_{1,\Omega}^2 &\le \|p_\epsilon - p_\epsilon^h(u_\epsilon)\|_{1,\Omega}^2 + \|p_\epsilon^h(u_\epsilon) - p_\epsilon^h\|_{1,\Omega}^2 \\ &\le Ch^2 + \|y_\epsilon^h - y_\epsilon^h(u_\epsilon)\|_{0,\Gamma}^2 \\ &\le Ch^2 + Ch_U^2.\end{aligned} \tag{4.16}$$

Combining (4.13), (4.14) and (4.16) we complete the proof. □

In Theorem 4.1, we provided the error estimate for the finite element approximation of the regularized BLT problem (2.9)-(2.11):

$$\epsilon\|u_\epsilon - u_\epsilon^h\|_{0,\Omega_U}^2 + \|y_\epsilon - y_\epsilon^h\|_{0,\Gamma}^2 + \|p_\epsilon - p_\epsilon^h\|_{1,\Omega}^2 = \mathcal{O}(h^2). \tag{4.17}$$

This result is valid for all $l \ge 0$, where l is the order of the finite element space for the control. Although it improves the result of the error estimate in [5], where the order of the error is

$$\epsilon\|u_\epsilon - u_\epsilon^h\|_{0,\Omega_U}^2 + \|y_\epsilon - y_\epsilon^h\|_{0,\Gamma}^2 = \mathcal{O}(h^{\frac{3}{2}}).$$

It is clear that this error estimate is not optimal, especially for the error of the state, i.e., $\|y_\epsilon - y_\epsilon^h\|_{0,\Gamma}^2$. The numerical results (see the next section) conform this conclusion.

In the following, we will try to improve the error estimate in Theorem 4.1 by considering the piecewise linear finite element approximation to control variable u_ϵ, while we again use the conforming piecewise linear finite element space to approximate the state y_ϵ and the costate p_ϵ. We will consider the case $Q_U = \{v \in L^2(\Omega_U),\ v \ge 0 \text{ a.e. in } \Omega_U\}$ in the following. For the other simple case where $Q_U = L^2(\Omega_U)$, the results of Theorem 4.2 can be improved (see Remark 4.3). In order to have the improved error estimate, we divide the domain Ω_U into three parts:

$$\begin{aligned}\Omega_U^+ &= \{\cup\tau_U :\ \tau_U \subset \Omega_U,\ u_\epsilon|_{\tau_U} > 0\}, \\ \Omega_U^0 &= \{\cup\tau_U :\ \tau_U \subset \Omega_U,\ u_\epsilon|_{\tau_U} = 0\}, \\ \Omega_U^b &= \Omega_U \backslash (\Omega_U^+ \cup \Omega_U^0).\end{aligned}$$

In the following, we assume that u_ϵ and $\mathcal{T}_U^h$ are regular such that $meas(\Omega_U^b) \le Ch_U$. This assumption can be satisfied in many practical cases. For example, when the free boundary Γ_0 is a curve with the finite length L, then $meas(\Omega_U^b) \le Ch_U L \le Ch_U$, because that Ω_U^b consists of the elements which intersect with the free boundary Γ_0.

Theorem 4.2. *Let* $(y_\epsilon, p_\epsilon, u_\epsilon)$ *be the solution of the problem* (2.9)-(2.11), *and* $(y_\epsilon^h, p_\epsilon^h, u_\epsilon^h)$ *be the solution of the problem* (3.2)-(3.4). *Let all conditions in Theorem 4.1 are valid. Moreover let* W_U^h *be piecewise linear finite element space, assume that* $u_\epsilon \in W^{1,\infty}(\Omega_U) \cap H^2(\Omega_U^+)$, $y_\epsilon \in W^{2,\infty}(\Omega)$, $p_\epsilon \in W^{1,\infty}(\Omega) \cap H^2(\Omega)$. *Then we have*

$$\epsilon\|u_\epsilon - u_\epsilon^h\|_{0,\Omega_U}^2 + \|y_\epsilon - y_\epsilon^h\|_{0,\Gamma}^2 + \|p_\epsilon - p_\epsilon^h\|_{0,\Omega}^2 \le C\epsilon^{-1}h^4 + Ch_U^3 + Ch^4|\ln h|^2. \tag{4.18}$$

Proof. Let $\pi_h : L^2(\Omega_U) \to W_U^h$ be the standard Lagrange interpolation operator. Then $\pi_h u_\epsilon \in Q_U^h$ for all $u_\epsilon \in Q_U$. Similar to Theorem 4.1, we have

$$\begin{aligned}
&\epsilon\|u_\epsilon - u_\epsilon^h\|_{0,\Omega_U}^2 + \|y_\epsilon^h - y_\epsilon^h(u_\epsilon)\|_{0,\Gamma}^2 \\
&= (B^*p_\epsilon + \epsilon u_\epsilon, u_\epsilon - u_\epsilon^h)_U + (B^*p_\epsilon^h(u_\epsilon) - B^*p_\epsilon, u_\epsilon - u_\epsilon^h)_U \\
&\quad +(B^*p_\epsilon^h + \epsilon u_\epsilon^h, u_\epsilon^h - \pi_h u_\epsilon)_U + (B^*p_\epsilon^h + \epsilon u_\epsilon^h, \pi_h u_\epsilon - u_\epsilon)_U \\
&\le 0 + \|B^*(p_\epsilon^h(u_\epsilon) - p_\epsilon)\|_{0,\Omega_U}\|u_\epsilon - u_\epsilon^h\|_{0,\Omega_U} + 0 + (B^*p_\epsilon^h + \epsilon u_\epsilon^h, \pi_h u_\epsilon - u_\epsilon)_U \\
&\le C(\delta)\epsilon^{-1}\|p_\epsilon^h(u_\epsilon) - p_\epsilon\|_{0,\Omega}^2 + C\delta\epsilon\|u_\epsilon - u_\epsilon^h\|_{0,\Omega_U}^2 + (B^*p_\epsilon + \epsilon u_\epsilon, \pi_h u_\epsilon - u_\epsilon)_U \\
&\quad +\epsilon(u_\epsilon^h - u_\epsilon, \pi_h u_\epsilon - u_\epsilon)_U + (B^*p_\epsilon^h - B^*p_\epsilon^h(u_\epsilon), \pi_h u_\epsilon - u_\epsilon)_U \\
&\quad +(B^*p_\epsilon^h(u_\epsilon) - B^*p_\epsilon, \pi_h u_\epsilon - u_\epsilon)_U \\
&\le C(\delta)\epsilon^{-1}\|p_\epsilon^h(u_\epsilon) - p_\epsilon\|_{0,\Omega}^2 + C\delta\epsilon\|u_\epsilon - u_\epsilon^h\|_{0,\Omega_U}^2 + (B^*p_\epsilon + \epsilon u_\epsilon, \pi_h u_\epsilon - u_\epsilon)_U \\
&\quad +C(\delta)\epsilon\|\pi_h u_\epsilon - u_\epsilon\|_{0,\Omega_U}^2 + C(\delta)\|\pi_h u_\epsilon - u_\epsilon\|_{0,\Omega_U}^2 + C\delta\|p_\epsilon^h - p_\epsilon^h(u_\epsilon)\|_{0,\Omega}^2,
\end{aligned} \tag{4.19}$$

where $(y_\epsilon^h(u_\epsilon), p_\epsilon^h(u_\epsilon))$ is the solution of the auxiliary equation (4.2)-(4.3), and δ is an arbitrary small positive number. Note that

$$\begin{aligned}
&(B^*p_\epsilon + \epsilon u_\epsilon, \pi u_\epsilon - u_\epsilon)_U \\
&= \int_{\Omega_U^+}(\epsilon u_\epsilon + B^*p_\epsilon)(\pi u_\epsilon - u_\epsilon) + \int_{\Omega_U^0}(\epsilon u_\epsilon + B^*p_\epsilon)(\pi u_\epsilon - u_\epsilon) \\
&\quad + \int_{\Omega_U^b}(\epsilon u_\epsilon + B^*p_\epsilon)(\pi u_\epsilon - u_\epsilon),
\end{aligned}$$

and

$$(\epsilon u_\epsilon + B^*p_\epsilon)|_{\Omega_U^+} = 0, \quad (\pi u_\epsilon - u_\epsilon)|_{\Omega_U^0} = 0.$$

From the definition of Ω_U^b we know that there exists at least one point $z_{\tau_U} \in \tau_U$ for each element $\tau_U \in \Omega_U^b$ such that $u(z_{\tau_U}) > 0$. Therefore we have $(\epsilon u_\epsilon + B^*p_\epsilon)(z_{\tau_U}) = 0$, and then

$$\begin{aligned}
&(B^*p_\epsilon + \epsilon u_\epsilon, \pi u_\epsilon - u_\epsilon)_U \\
&= \int_{\Omega_U^b}(\epsilon u_\epsilon + B^*p_\epsilon)(\pi u_\epsilon - u_\epsilon) \\
&= \sum_{\tau_U \in \Omega_U^b}\int_{\tau_U}(\epsilon u_\epsilon + B^*p_\epsilon - (\epsilon u_\epsilon + B^*p_\epsilon)(z_{\tau_U}))(\pi u_\epsilon - u_\epsilon) \\
&\le C\sum_{\tau_U \in \Omega_U^b} h_{\tau_U}^2|\epsilon u_\epsilon + B^*p_\epsilon|_{1,\infty,\tau_U}|u_\epsilon|_{1,\infty,\tau_U} meas(\Omega_U^b) \le Ch_U^3.
\end{aligned} \tag{4.20}$$

Similarly, it can be concluded that

$$\begin{aligned}\|\pi_h u_\epsilon - u_\epsilon\|^2_{0,\Omega_U} &= \|\pi_h u_\epsilon - u_\epsilon\|^2_{0,\Omega_U^+} + \|\pi_h u_\epsilon - u_\epsilon\|^2_{0,\Omega_U^0} + \|\pi_h u_\epsilon - u_\epsilon\|^2_{0,\Omega_U^b} \\ &\le Ch_U^4 \|u_\epsilon\|^2_{2,\Omega_U^+} + 0 + Ch_U^2 \|u_\epsilon\|^2_{1,\infty,\Omega_U^b} meas(\Omega_U^b) \le Ch_U^3. \end{aligned} \tag{4.21}$$

Furthermore, it follows from (3.3) and (4.3) that

$$\|p_\epsilon^h - p_\epsilon^h(u_\epsilon)\|_{0,\Omega} \le \|p_\epsilon^h - p_\epsilon^h(u_\epsilon)\|_{1,\Omega} \le C\|y_\epsilon^h - y_\epsilon^h(u_\epsilon)\|_{0,\partial\Omega}. \tag{4.22}$$

Combining (4.19)-(4.22) and (4.12) we have

$$\epsilon\|u_\epsilon - u_\epsilon^h\|^2_{0,\Omega_U} + \|y_\epsilon^h - y_\epsilon^h(u_\epsilon)\|^2_{0,\Gamma} \le C\epsilon^{-1}h^4 + Ch_U^3. \tag{4.23}$$

Noting that $y_\epsilon^h(u_\epsilon)$ is the standard finite element solution of y_ϵ, we have that (see, e.g., [1])

$$\|y_\epsilon - y_\epsilon^h(u_\epsilon)\|_{0,\Gamma} \le C\|y_\epsilon - y_\epsilon^h(u_\epsilon)\|_{0,\infty,\Omega} \le Ch^2|\ln h|\|y_\epsilon\|_{2,\infty,\Omega}.$$

Then similar to Theorem 4.1, we have that

$$\begin{aligned}\|y_\epsilon - y_\epsilon^h\|^2_{0,\Gamma} &\le \|y_\epsilon - y_\epsilon^h(u_\epsilon)\|^2_{0,\Gamma} + \|y_\epsilon^h(u_\epsilon) - y_\epsilon^h\|^2_{0,\Gamma} \\ &\le Ch^4|\ln h|^2 + C\epsilon^{-1}h^4 + Ch_U^3, \end{aligned} \tag{4.24}$$

and

$$\begin{aligned}\|p_\epsilon - p_\epsilon^h\|^2_{0,\Omega} &\le \|p_\epsilon - p_\epsilon^h(u_\epsilon)\|^2_{0,\Omega} + \|p_\epsilon^h(u_\epsilon) - p_\epsilon^h\|^2_{0,\Omega} \\ &\le Ch^4 + C\|y_\epsilon^h(u_\epsilon) - y_\epsilon^h\|^2_{0,\Gamma} \\ &\le Ch^4|\ln h|^2 + C\epsilon^{-1}h^4 + Ch_U^3, \end{aligned} \tag{4.25}$$

Summing up, (4.18) follows from (4.23)-(4.25). □

Remark 4.3. Although Theorem 4.2 improved the result of Theorem 4.1, but it is regretful that it is an improvement only when ϵ is not too small, e.g., ϵ should be larger than h^2. Especially, when $\epsilon \ge C$, the error order should be $\mathcal{O}(h^2|\ln h| + h_U^{3/2})$ instead of $\mathcal{O}(h + h_U)$. Here the suboptimal error order $\mathcal{O}(h_U^{3/2})$ is caused by the singularity of the solution u_ϵ near the free boundary. When $Q_U = L^2(\Omega_U)$, there is no free boundary, and we can assume that $u \in H^2(\Omega_U)$. Then (4.20) and (4.21) can be improved to

$$B^* p_\epsilon + \epsilon u_\epsilon = 0$$

and

$$\|\pi_h u_\epsilon - u_\epsilon\|_{0,\Omega_U} \le Ch_U^2 \|u_\epsilon\|_{2,\Omega_U}.$$

Thus, the error order in Theorem 4.2 can be improved to $\mathcal{O}(\epsilon^{-\frac{1}{2}}h^2 + h^2|\ln h| + h_U^2)$.

5. Numerical Examples

In this section, we presented some numerical examples to verify the estimates of the finite element approximation in Section 3. For the optimal control problem, the state and the control are more interested quantity than the co-state due to its importance in practice. Therefore in

Table 5.1: L^2-errors of the state y_ϵ and the control u_ϵ for Example 5.1, using piecewise constant finite element space for the control and piecewise linear finite element space for the state.

ϵ		# mesh nodes			order
		277	1055	4117	
0.1	$\|u_\epsilon^h - u_\epsilon\|_{L^2(\Omega)}$	0.0706998	0.0354385	0.0177333	1
	$\|y_\epsilon^h - y_\epsilon\|_{L^2(\partial\Omega)}$	0.00166397	0.000429685	0.000102564	2
0.01	$\|u_\epsilon^h - u_\epsilon\|_{L^2(\Omega)}$	0.0712926	0.0355151	0.0177554	1
	$\|y_\epsilon^h - y_\epsilon\|_{L^2(\partial\Omega)}$	0.00170581	0.000440191	0.000099923	2
0.001	$\|u_\epsilon^h - u_\epsilon\|_{L^2(\Omega)}$	0.0739751	0.035851	0.0178042	1
	$\|y_\epsilon^h - y_\epsilon\|_{L^2(\partial\Omega)}$	0.00187942	0.000477981	0.000121379	2

Table 5.2: L^2-errors of the state y_ϵ and the control u_ϵ for Example 5.1, using piecewise linear finite element space for both the control and the state.

ϵ		# mesh nodes			order
		277	1055	4117	
0.1	$\|u_\epsilon^h - u_\epsilon\|_{L^2(\Omega)}$	0.00921624	0.0037779	0.00123061	1.62
	$\|y_\epsilon^h - y_\epsilon\|_{L^2(\partial\Omega)}$	0.001674	0.000418599	0.000110845	2
0.01	$\|u_\epsilon^h - u_\epsilon\|_{L^2(\Omega)}$	0.0128337	0.0044474	0.00135877	1.71
	$\|y_\epsilon^h - y_\epsilon\|_{L^2(\partial\Omega)}$	0.00171644	0.000430845	0.000112126	2
0.001	$\|u_\epsilon^h - u_\epsilon\|_{L^2(\Omega)}$	0.0226521	0.00673849	0.00186549	1.85
	$\|y_\epsilon^h - y_\epsilon\|_{L^2(\partial\Omega)}$	0.0018967	0.000476881	0.000121028	2

the following numerical examples, we only present the results of the state and the control, while the data for the co-state were omitted.

First we examined the convergence order of the finite element solution for the regularized problem. The problem under consideration is as

$$\min_{u_\epsilon \in Q_U} \left\{ \frac{1}{2}\|y_\epsilon - g_1\|^2_{L^2(\Gamma)} + \frac{\epsilon}{2}\|u_\epsilon\|^2_{L^2(\Omega)} \right\} \tag{5.1}$$

subjected to

$$-\Delta y_\epsilon + y_\epsilon = u_\epsilon + f, \quad \text{in } \Omega, \tag{5.2}$$

$$\frac{\partial y_\epsilon}{\partial n} = g_2, \quad \text{on } \partial\Omega, \tag{5.3}$$

where

$$Q_U = \{v \in L^2(\Omega) : \ v \geq 0\}, \quad \Omega = \{(x_1, x_2) : \ {x_1}^2 + {x_2}^2 \leq 1\}.$$

Then the co-state equation of the problem is

$$-\Delta p_\epsilon + p_\epsilon = 0 \quad \text{in } \Omega,$$
$$\frac{\partial p_\epsilon}{\partial n} = y_\epsilon - g_1 \quad \text{on } \partial\Omega.$$

The right hand side term f in the constrain equation (5.2) is introduced to make an exact solution available. In the following numerical examples, we used the three meshes, obtained by sequentially refined a quasi-uniform background mesh with nodes number as 277, 1055 and 4117.

Table 5.3: The error of $(y_\epsilon^h, u_\epsilon^h)$ to (y, u) with ϵ approaching zero.

ϵ	$h = 0.1$		$h = 0.05$	
	$\|u_\epsilon^h - u\|_{L^2(\Omega)}$	$\|y_\epsilon^h - y\|_{L^2(\partial\Omega)}$	$\|u_\epsilon^h - u\|_{L^2(\Omega)}$	$\|y_\epsilon^h - y\|_{L^2(\partial\Omega)}$
2^{-1}	1.43608	0.624236	1.43607	0.625114
2^{-2}	1.21323	0.450697	1.21318	0.451689
2^{-3}	0.970780	0.312104	0.970063	0.313135
2^{-4}	0.745611	0.202724	0.745531	0.203720
2^{-5}	0.553699	0.124724	0.554001	0.125660
2^{-6}	0.404896	0.0730709	0.406007	0.0739797
2^{-7}	0.298441	0.0410194	0.300634	0.0419472
2^{-8}	0.229740	0.0220504	0.232178	0.0230450
2^{-9}	0.192386	0.0112031	0.194608	0.0122475
2^{-10}	0.177602	0.00518454	0.178179	0.00626051

Example 5.1. In this example, we consider the problem (5.1) -(5.3) with

$$\begin{aligned} f(x_1, x_2) &= 3y_\epsilon(x_1, x_2) - u_\epsilon(x_1, x_2), \\ g_1(x_1, x_2) &= \epsilon x u_\epsilon + y_\epsilon(x_1, x_2), \\ g_2(x_1, x_2) &= (x_1 + x_2)\cos(x_1 + x_2), \end{aligned}$$

and the exact solutions is

$$u_\epsilon(x_1, x_2) = \max\left\{e^{x_1} - e^{-x_1}, 0\right\}, \quad y_\epsilon(x_1, x_2) = \sin(x_1 + x_2).$$

We firstly used the piecewise constant finite element space and the piecewise linear finite element space to approximate the control u_ϵ and the state y_ϵ, respectively. In Table 5.1, the L^2 error of the control u_ϵ and the state y_ϵ are presented. The L^2 error of u_ϵ is of order $\mathcal{O}(h)$, while the L^2 error of y_ϵ is of order $\mathcal{O}(h^2)$. The accuracy order is independent of ϵ, though the magnitude of the error is slightly larger with smaller ϵ.

Then we approximated using piecewise linear finite element spaces for both the control and the state. The error of the control u_ϵ and the state y_ϵ were listed in Table 5.2. It is shown that again the error of y_ϵ is of order $\mathcal{O}(h^2)$, while the accuracy order of u_ϵ is improved to be over 1.6.

Example 5.2. In this example, we examine the dependence of the approximation quality the numerical solution $(y_\epsilon^h, u_\epsilon^h)$ of the regularized problem (3.2)-(3.4) to the solution (y, u) of the original problem without regularization, (2.1) with the boundary conditions (2.4) and (2.5), on the penalty parameter ϵ when ϵ is going to zero. We set $D = I$ and $\mu = 1$, Ω and Q_U are same as Example 5.1. We set

$$\begin{aligned} u(x_1, x_2) &= \max\{3\sin(x_1 + x_2), 0\}, \\ y(x_1, x_2) &= \sin(x_1 + x_2), \\ f(x_1, x_2) &= 3y(x_1, x_2) - u(x_1, x_2), \\ g_1(x_1, x_2) &= y(x_1, x_2), \\ g_2(x_1, x_2) &= (x_1 + x_2)\cos(x_1 + x_2). \end{aligned}$$

In Table 5.3 and Fig. 5.1, we listed the error of $(y_\epsilon^h, u_\epsilon^h)$ as the approximation of (y, u) with decreasing ϵ. It is shown that $(y_\epsilon^h, u_\epsilon^h)$ converge to (y, u) as ϵ is going to zero, and the

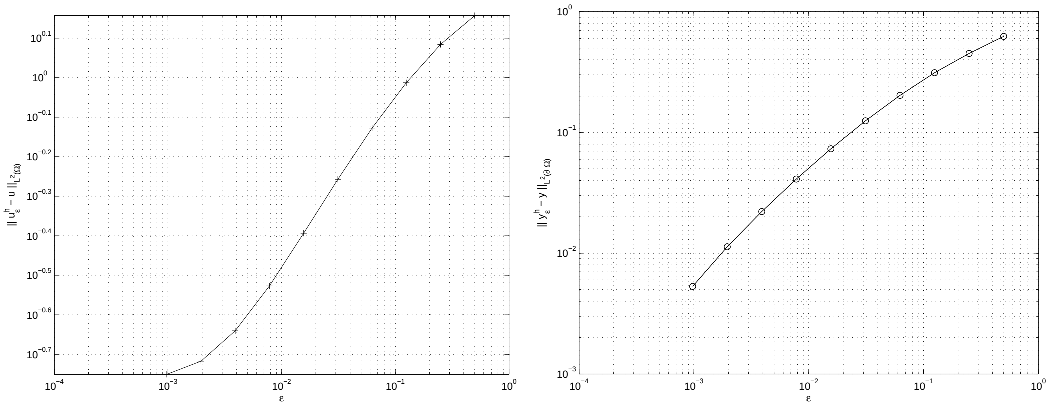

Fig. 5.1. The dependence of error on the regularization parameter ϵ.

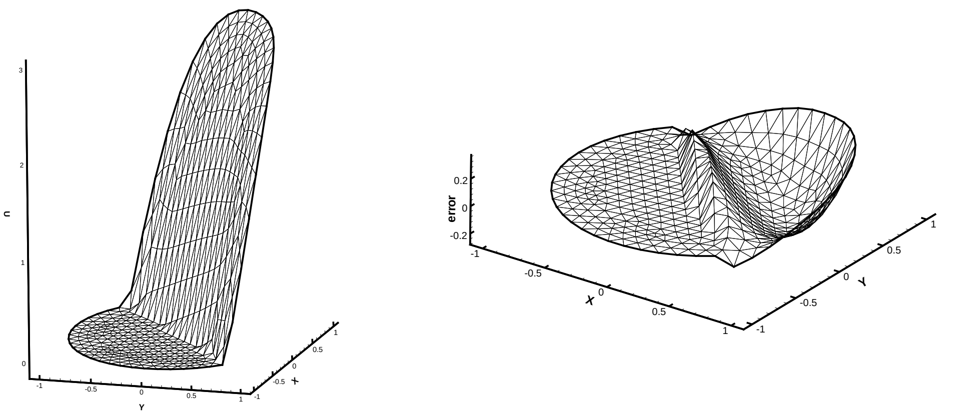

Fig. 5.2. The surface of the exact solution u (left) and the error distribution of the approximated solution u_ϵ^h to u with $\epsilon = 2^{-10}$ and $h = 0.1$ (right).

convergence order of the state is increasing upto 1, but there are no positive convergence order for the control with respected to ϵ. In the comparison of the data obtained by using $h = 0.1$ and $h = 0.05$ in Table 5.3, it can be found that the error can not be reduced by mesh refinement. It is indicated that for this example, the essential part of the error is introduced by the regularization of the original problem instead of the finite element approximation. In Fig. 5.2, the figures of the exact solution u and the error distribution of the approximation u_ϵ^h with $\epsilon = 2^{-10}$ and $h = 0.1$ were plotted to show the effects introduced by the regularization on the solution of the original problem.

6. Discussion

In this paper, we provide an improved a priori error estimate for the finite element approximation of the regularized BLT problem, and some numerical examples are presented to demonstrate our theoretical results. There are many important issues that remain to be studied and which will be dealt with in a sequel to the present paper. There, the focus will be on the a posteriori error estimate and adaptive finite element method. They may improve the computing efficiency because there will have singularity near the source and interface of the medium.

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