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OPTIMAL CONTROL OF THE LAPLACE–BELTRAMI OPERATOR ON COMPACT SURFACES: CONCEPT AND NUMERICAL TREATMENT*

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Abstract

We consider optimal control problems of elliptic PDEs on hypersurfaces Γ in $\mathbb{R}^n$ for $n = 2, 3$. The leading part of the PDE is given by the Laplace-Beltrami operator, which is discretized by finite elements on a polyhedral approximation of Γ. The discrete optimal control problem is formulated on the approximating surface and is solved numerically with a semi-smooth Newton algorithm. We derive optimal a priori error estimates for problems including control constraints and provide numerical examples confirming our analytical findings.

Mathematics subject classification: 58J32, 49J20, 49M15.
Key words: Elliptic optimal control problem, Laplace-Beltrami operator, Surfaces, Control constraints, Error estimates, Semi-smooth Newton method.

1. Introduction

We are interested in the numerical treatment of the following linear-quadratic optimal control problem on a n-dimensional, sufficiently smooth hypersurface $\Gamma \subset \mathbb{R}^{n+1}$, $n = 1, 2$.

$$\begin{aligned} \min_{u\in L^2(\Gamma),\, y\in H^1(\Gamma)} J(u,y) &= \frac{1}{2}\|y-z\|^2_{L^2(\Gamma)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Gamma)} \\ &\text{subject to} \quad u \in U_{ad} \quad \text{and} \\ &\int_\Gamma \nabla_\Gamma y \nabla_\Gamma \varphi + \mathbf{c} y\varphi \,\mathrm{d}\Gamma = \int_\Gamma u\varphi \,\mathrm{d}\Gamma \,, \forall \varphi \in H^1(\Gamma) \end{aligned} \tag{1.1}$$

with $U_{ad} = \{v \in L^2(\Gamma) \mid a \le v \le b\}$, $a < b \in \mathbb{R}$. For simplicity we will assume Γ to be compact and $\mathbf{c} = 1$. In section 4 we briefly investigate the case $\mathbf{c} = 0$, in section 5 we give an example on a surface with boundary.

Problem (1.1) may serve as a mathematical model for the optimal distribution of surfactants on a biomembrane Γ with regard to achieving a prescribed desired concentration z of a quantity y.

It follows by standard arguments that (1.1) admits a unique solution $u \in U_{ad}$ with unique associated state $y = y(u) \in H^2(\Gamma)$.

Our numerical approach uses variational discretization applied to (1.1), see [9] and [10], on a discrete surface Γ^h approximating Γ. The discretization of the state equation in (1.1) is achieved

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by the finite element method proposed in [4], where a priori error estimates for finite element approximations of the Poisson problem for the Laplace-Beltrami operator are provided. Let us mention that uniform estimates are presented in [2], and steps towards a posteriori error control for elliptic PDEs on surfaces are taken by Demlow and Dziuk in [3]. For alternative approaches for the discretization of the state equation by finite elements see the work of Burger [1]. Finite element methods on moving surfaces are developed by Dziuk and Elliott in [5]. To the best of the authors knowledge, the present paper contains the first attempt to treat optimal control problems on surfaces.

We assume that Γ is of class C^2. As an embedded, compact hypersurface in $\mathbb{R}^{n+1}$ it is orientable with an exterior unit normal field ν and hence the zero level set of a signed distance function d such that

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

Further, there exists an neighborhood $\mathcal{N} \subset \mathbb{R}^{n+1}$ of Γ, such that d is also of class C^2 on $\mathcal{N}$ and the projection

$$a : \mathcal{N} \to \Gamma\,, \quad a(x) = x - d(x)\nabla d(x) \tag{1.2}$$

is unique, see e.g. [6, Lemma 14.16]. Note that $\nabla d(x) = \nu(a(x))$.

Using a we can extend any function $\phi : \Gamma \to \mathbb{R}$ to $\mathcal{N}$ as $\bar{\phi}(x) = \phi(a(x))$. This allows us to represent the surface gradient in global exterior coordinates $\nabla_\Gamma \phi = (I - \nu\nu^T)\nabla\bar{\phi}$, with the euclidean projection $(I - \nu\nu^T)$ onto the tangential space of Γ.

We use the Laplace-Beltrami operator $\Delta_\Gamma = \nabla_\Gamma \cdot \nabla_\Gamma$ in its weak form i.e. $\Delta_\Gamma : H^1(\Gamma) \to H^1(\Gamma)^*$

$$y \mapsto -\int_\Gamma \nabla_\Gamma y \nabla_\Gamma(\,\cdot\,)\,\mathrm{d}\Gamma \in H^1(\Gamma)^*\,.$$

Let S denote the prolongated restricted solution operator of the state equation

$$S : L^2(\Gamma) \to L^2(\Gamma)\,, \quad u \mapsto y \qquad -\Delta_\Gamma y + \mathbf{c}y = u\,,$$

which is compact and constitutes a linear homeomorphism onto $H^2(\Gamma)$, see [4, 1. Theorem].

By standard arguments we get the following necessary (and here also sufficient) conditions for optimality of $u \in U_{ad}$

$$\begin{aligned} &\langle \nabla_u J(u, y(u)), v - u\rangle_{L^2(\Gamma)} \\ =&\langle \alpha u + S^*(Su - z), v - u\rangle_{L^2(\Gamma)} \geq 0 \quad \forall v \in U_{ad}\,. \end{aligned} \tag{1.3}$$

We rewrite (1.3) as

$$u = \mathrm{P}_{U_{ad}}\left(-\frac{1}{\alpha}S^*(Su - z)\right)\,, \tag{1.4}$$

where $\mathrm{P}_{U_{ad}}$ denotes the L^2-orthogonal projection onto U_{ad}.

2. Discretization

We now discretize (1.1) using an approximation Γ^h to Γ which is globally of class $C^{0,1}$. Following Dziuk, we consider polyhedral $\Gamma^h = \bigcup_{i \in I_h} T_h^i$ consisting of triangles T_h^i with corners on Γ, whose maximum diameter is denoted by h. With FEM error bounds in mind we assume the family of triangulations Γ^h to be regular in the usual sense that the angles of all triangles are bounded away from zero uniformly in h.

We assume for Γ^h that $a(\Gamma^h) = \Gamma$, with a from (1.2). For small $h > 0$ the projection a also is injective on Γ^h. In order to compare functions defined on Γ^h with functions on Γ we use a to lift a function $y \in L^2(\Gamma^h)$ to Γ

$$y^l(a(x)) = y(x) \quad \forall x \in \Gamma^h ,$$

and for $y \in L^2(\Gamma)$ and sufficiently small $h > 0$ we define the inverse lift

$$y_l(x) = y(a(x)) \quad \forall x \in \Gamma^h .$$

For small mesh parameters h the lift operation $(\cdot)_l : L^2(\Gamma) \to L^2(\Gamma^h)$ defines a linear homeomorphism with inverse $(\cdot)^l$. Moreover, there exists $c_{\text{int}} > 0$ such that

$$1 - c_{\text{int}} h^2 \leq \|(\cdot)_l\|^2_{\mathcal{L}(L^2(\Gamma),L^2(\Gamma^h))}, \|(\cdot)^l\|^2_{\mathcal{L}(L^2(\Gamma^h),L^2(\Gamma))} \leq 1 + c_{\text{int}} h^2 , \tag{2.1}$$

as the following lemma shows.

Lemma and Definition 2.1. *Denote by* $\frac{\mathrm{d}\Gamma}{\mathrm{d}\Gamma^h}$ *the Jacobian of* $a|_{\Gamma^h} : \Gamma^h \to \Gamma$, *i.e.*

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}\Gamma^h} = |\det(M)|,$$

where $M \in \mathbb{R}^{n \times n}$ *represents the Derivative* $\mathrm{d}a(x) : T_x\Gamma^h \to T_{a(x)}\Gamma$ *with respect to arbitrary orthonormal bases of the respective tangential space. For small* $h > 0$ *there holds*

$$\sup_{\Gamma} \left| 1 - \frac{\mathrm{d}\Gamma}{\mathrm{d}\Gamma^h} \right| \leq c_{\text{int}} h^2 .$$

Now let $\frac{\mathrm{d}\Gamma^h}{\mathrm{d}\Gamma}$ *denote* $|\det(M^{-1})|$, *so that by the change of variable formula*

$$\left| \int_{\Gamma^h} v_l \,\mathrm{d}\Gamma^h - \int_{\Gamma} v \,\mathrm{d}\Gamma \right| = \left| \int_{\Gamma} v \frac{\mathrm{d}\Gamma^h}{\mathrm{d}\Gamma} - v \,\mathrm{d}\Gamma \right| \leq c_{\text{int}} h^2 \|v\|_{L^1(\Gamma)} .$$

Proof. see [5, Lemma 5.1] □

Problem (1.1) is approximated by the following sequence of optimal control problems

$$\min_{u \in L^2(\Gamma^h),\, y \in H^1(\Gamma^h)} J(u,y) = \frac{1}{2}\|y - z_l\|^2_{L^2(\Gamma^h)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Gamma^h)} \\ \text{subject to} \quad u \in U^h_{ad} \text{ and } \quad y = S_h u , \tag{2.2}$$

with $U^h_{ad} = \left\{ v \in L^2(\Gamma^h) \mid a \leq v \leq b \right\}$, i.e. the mesh parameter h enters into U_{ad} only through Γ^h . Problem (2.2) may be regarded as the extension of variational discretization introduced in [9] to optimal control problems on surfaces.

In [4] it is explained, how to implement a discrete solution operator $S_h : L^2(\Gamma^h) \to L^2(\Gamma^h)$, such that

$$\|(\cdot)^l S_h (\cdot)_l - S\|_{\mathcal{L}(L^2(\Gamma),L^2(\Gamma))} \leq C_{\text{FE}} h^2 , \tag{2.3}$$

which we will use throughout this paper. See in particular [4, Eq. (6)] and [4, Lemma 7]. For the convenience of the reader we briefly sketch the method. Consider the space

$$V_h = \left\{ \varphi \in C^0\left(\Gamma^h\right) \;\middle|\; \forall i \in I_h : \varphi|_{T^i_h} \in \mathcal{P}^1(T^i_h) \right\} \subset H^1(\Gamma^h)$$

of piecewise linear, globally continuous functions on Γ^h. For some $u \in L^2(\Gamma)$, to compute $y_h^l = (\cdot)^l S_h(\cdot)_l u$ solve

$$\int_{\Gamma^h} \nabla_{\Gamma^h} y_h \nabla_{\Gamma^h} \varphi_i + \mathbf{c} y_h \varphi_i \,\mathrm{d}\Gamma^h = \int_{\Gamma^h} u_l \varphi_i \,\mathrm{d}\Gamma^h \,, \quad \forall \varphi \in V_h$$

for $y_h \in V_h$. We choose $L^2(\Gamma^h)$ as control space, because in general we cannot evaluate $\int_\Gamma v \,\mathrm{d}\Gamma$ exactly, whereas the expression $\int_{\Gamma^h} v_l \,\mathrm{d}\Gamma^h$ for piecewise polynomials v_l can be computed up to machine accuracy. Also, the operator S_h is self-adjoint, while $((\cdot)^l S_h(\cdot)_l)^* = (\cdot)_l{}^* S_h (\cdot)^{l^*}$ is not. The adjoint operators of $(\cdot)_l$ and $(\cdot)^l$ have the shapes

$$\forall v \in L^2(\Gamma^h) : \; ((\cdot)_l)^* v = \frac{\mathrm{d}\Gamma^h}{\mathrm{d}\Gamma} v^l \,, \quad \forall v \in L^2(\Gamma) : \; ((\cdot)^l)^* v = \frac{\mathrm{d}\Gamma}{\mathrm{d}\Gamma^h} v_l \,, \tag{2.4}$$

hence evaluating $(\cdot)_l{}^*$ and $(\cdot)^{l^*}$ requires knowledge of the Jacobians $\frac{\mathrm{d}\Gamma^h}{\mathrm{d}\Gamma}$ and $\frac{\mathrm{d}\Gamma}{\mathrm{d}\Gamma^h}$ which may not be known analytically.

Similar to (1.1), problem (2.2) possesses a unique solution $u_h \in U_{ad}^h$ which satisfies

$$u_h = \mathrm{P}_{U_{ad}^h} \left(-\frac{1}{\alpha} p_h(u_h) \right) . \tag{2.5}$$

Here $P_{U_{ad}^h} : L^2(\Gamma^h) \to U_{ad}^h$ is the $L^2(\Gamma^h)$-orthogonal projection onto U_{ad}^h and for $v \in L^2(\Gamma^h)$ the adjoint state is $p_h(v) = S_h^*(S_h v - z_l) \in H^1(\Gamma^h)$.

Observe that the projections $\mathrm{P}_{U_{ad}}$ and $\mathrm{P}_{U_{ad}^h}$ coincide with the point-wise projection $\mathrm{P}_{[a,b]}$ on Γ and Γ^h, respectively, and hence

$$\left(\mathrm{P}_{U_{ad}^h} (v_l) \right)^l = \mathrm{P}_{U_{ad}} (v) \tag{2.6}$$

for any $v \in L^2(\Gamma)$.

Let us now investigate the relation between the optimal control problems (1.1) and (2.2).

Theorem 2.2 (Order of Convergence) *Let $u \in L^2(\Gamma)$, $u_h \in L^2(\Gamma^h)$ be the solutions of* (1.1) *and* (2.2)*, respectively. Then for sufficiently small $h > 0$ there holds*

$$\begin{aligned} &\alpha \left\| u_h^l - u \right\|_{L^2(\Gamma)}^2 + \left\| y_h^l - y \right\|_{L^2(\Gamma)}^2 \\ \le &\frac{1 + c_{\mathrm{int}} h^2}{1 - c_{\mathrm{int}} h^2} \left(\frac{1}{\alpha} \left\| \left((\cdot)^l S_h^* (\cdot)_l - S^* \right) (y - z) \right\|_{L^2(\Gamma)}^2 \cdots + \left\| \left((\cdot)^l S_h (\cdot)_l - S \right) u \right\|_{L^2(\Gamma)}^2 \right), \end{aligned} \tag{2.7}$$

with $y = Su$ and $y_h = S_h u_h$.

Proof. From (2.6) it follows that the projection of $-\left(\frac{1}{\alpha} p(u)\right)_l$ onto U_{ad}^h is u_l

$$u_l = \mathrm{P}_{U_{ad}^h} \left(-\frac{1}{\alpha} p(u)_l \right) ,$$

which we insert into the necessary condition of (2.2). This gives

$$\langle \alpha u_h + p_h(u_h), u_l - u_h \rangle_{L^2(\Gamma^h)} \ge 0 \,.$$

On the other hand u_l is the $L^2(\Gamma^h)$-orthogonal projection of $-\frac{1}{\alpha} p(u)_l$, thus

$$\langle -\frac{1}{\alpha} p(u)_l - u_l, u_h - u_l \rangle_{L^2(\Gamma^h)} \le 0 \,.$$

Adding these inequalities yields

$$
\begin{aligned}
&\alpha\|u_l - u_h\|^2_{L^2(\Gamma^h)} \\
&\le \langle (p_h(u_h) - p(u)_l)\,, u_l - u_h\rangle_{L^2(\Gamma^h)} \\
&= \langle p_h(u_h) - S_h^*(y-z)_l, u_l - u_h\rangle_{L^2(\Gamma^h)} + \langle S_h^*(y-z)_l - p(u)_l, u_l - u_h\rangle_{L^2(\Gamma^h)}\,.
\end{aligned}
$$

The first addend is estimated via

$$
\begin{aligned}
&\langle p_h(u_h) - S_h^*(y-z)_l, u_l - u_h\rangle_{L^2(\Gamma^h)} \\
=&\ \langle y_h - y_l, S_h u_l - y_h\rangle_{L^2(\Gamma^h)} \\
=& - \|y_h - y_l\|^2_{L^2(\Gamma^h)} + \langle y_h - y_l, S_h u_l - y_l\rangle_{L^2(\Gamma^h)} \\
\le& - \frac{1}{2}\|y_h - y_l\|^2_{L^2(\Gamma^h)} + \frac{1}{2}\|S_h u_l - y_l\|^2_{L^2(\Gamma^h)}.
\end{aligned}
$$

The second addend satisfies

$$
\begin{aligned}
&\langle S_h^*(y-z)_l - p(u)_l, u_l - u_h\rangle_{L^2(\Gamma^h)} \\
\le&\ \frac{\alpha}{2}\|u_l - u_h\|^2_{L^2(\Gamma^h)} + \frac{1}{2\alpha}\|S_h^*(y-z)_l - p(u)_l\|^2_{L^2(\Gamma^h)}.
\end{aligned}
$$

Together this yields

$$
\begin{aligned}
&\alpha\|u_l - u_h\|^2_{L^2(\Gamma^h)} + \|y_h - y_l\|^2_{L^2(\Gamma^h)} \\
\le& \frac{1}{\alpha}\|S_h^*(y-z)_l - p(u)_l\|^2_{L^2(\Gamma^h)} + \|S_h u_l - y_l\|^2_{L^2(\Gamma^h)}.
\end{aligned}
$$

The claim follows using (2.1) for sufficiently small $h > 0$.

Because both S and S_h are self-adjoint, quadratic convergence follows directly from (2.7). For operators that are not self-adjoint one can use

$$
\|(\cdot)_l{}^* S_h^* (\cdot)^{l*} - S^*\|_{\mathcal{L}(L^2(\Gamma),L^2(\Gamma))} \le C_{\mathrm{FE}} h^2\,. \tag{2.8}
$$

which is a consequence of (2.3). Eq. (2.4) and Lemma 2.1 imply

$$
\begin{aligned}
&\|((\cdot)_l)^* - (\cdot)^l\|_{\mathcal{L}(L^2(\Gamma^h),L^2(\Gamma))} \le c_{\mathrm{int}} h^2, \\
&\|((\cdot)^l)^* - (\cdot)_l\|_{\mathcal{L}(L^2(\Gamma),L^2(\Gamma^h))} \le c_{\mathrm{int}} h^2.
\end{aligned} \tag{2.9}
$$

Combine (2.7) with (2.8) and (2.9) to prove quadratic convergence for arbitrary linear elliptic state equations.

3. Implementation

In order to solve (2.5) numerically, we proceed as in [9] using the finite element techniques for PDEs on surfaces developed in [4] combined with the semi-smooth Newton techniques from [7] and [12] applied to the equation

$$
G_h(u_h) = \left(u_h - \mathrm{P}_{[a,b]}\left(-\frac{1}{\alpha} p_h(u_h)\right)\right) = 0\,. \tag{3.1}
$$

Since the operator p_h continuously maps $v \in L^2(\Gamma^h)$ into $H^1(\Gamma^h)$, Equation (3.1) is semismooth and thus is amenable to a semismooth Newton method. The generalized derivative of G_h is given by

$$DG_h(u) = \left(I + \frac{\chi}{\alpha} S_h^* S_h\right),$$

where $\chi : \Gamma^h \to \{0,1\}$ denotes the indicator function of the inactive set $\mathcal{I}(-\frac{1}{\alpha}p_h(u)) = \left\{\gamma \in \Gamma^h \;\middle|\; a < -\frac{1}{\alpha}p_h(u)[\gamma] < b\right\}$

$$\chi = \begin{cases} 1 \text{ on } \mathcal{I}(-\frac{1}{\alpha}p_h(u)) \subset \Gamma^h \\ 0 \text{ elsewhere on } \Gamma^h \end{cases},$$

which we use both as a function and as the operator $\chi : L^2(\Gamma^h) \to L^2(\Gamma^h)$ defined as the point-wise multiplication with the function χ. A step of the semi-smooth Newton method for (3.1) then reads

$$\left(I + \frac{\chi}{\alpha} S_h^* S_h\right) u^+ = -G_h(u) + DG_h(u)u = \mathrm{P}_{[a,b]}\left(-\frac{1}{\alpha}p_h(u)\right) + \frac{\chi}{\alpha} S_h^* S_h u\,.$$

Given u the next iterate u^+ is computed by performing three steps

Algorithm 3.1. *1. Set* $((1-\chi)\,u^+)[\gamma] = \left((1-\chi)\mathrm{P}_{[a,b]}\left(-\frac{1}{\alpha}p_h(u)\right)\right)[\gamma]$, *which is either* a *or* b, *depending on* $\gamma \in \Gamma_h$.

2. Solve

$$\left(I + \frac{\chi}{\alpha} S_h^* S_h\right) \chi u^+ = \frac{\chi}{\alpha}\left(S_h^* z_l - S_h^* S_h\,(1-\chi)\,u^+\right)$$

for χu^+ *by CG iteration over* $L^2(\mathcal{I}(-\frac{1}{\alpha}p_h(u))$.

3. Set $u^+ = \chi u^+ + (1-\chi)u^+$.

Details can be found in [11] .

4. The Case $\mathbf{c} = 0$

In this section we investigate the case $\mathbf{c} = 0$ which corresponds to a stationary, purely diffusion driven process. Since Γ has no boundary, in this case total mass must be conserved, i.e. the state equation admits a solution only for controls with mean value zero. For such a control the state is uniquely determined up to a constant. Thus the admissible set U_{ad} has to be changed to

$$U_{ad} = \left\{v \in L^2(\Gamma) \;\; a \le v \le b\right\} \cap L_0^2(\Gamma)\,, \text{ where } L_0^2(\Gamma) := \left\{v \in L^2(\Gamma) \;\middle|\; \int_\Gamma v \,\mathrm{d}\Gamma = 0\right\},$$

and $a < 0 < b$. Problem (1.1) then admits a unique solution (u, y) and there holds $\int_\Gamma y \,\mathrm{d}\Gamma = \int_\Gamma z \,\mathrm{d}\Gamma$. W.l.o.g we assume $\int_\Gamma z \,\mathrm{d}\Gamma = 0$ and therefore only need to consider states with mean value zero. The state equation now reads $y = \tilde{S}u$ with the solution operator $\tilde{S} : L_0^2(\Gamma) \to L_0^2(\Gamma)$ of the equation $-\Delta_\Gamma y = u$, $\int_\Gamma y \,\mathrm{d}\Gamma = 0$.

Using the injection $L_0^2(\Gamma) \xrightarrow{\imath} L^2(\Gamma)$, $\tilde{S}$ is prolongated as an operator $S : L^2(\Gamma) \to L^2(\Gamma)$ by $S = \imath\tilde{S}\imath^*$. The adjoint $\imath^* : L^2(\Gamma) \to L_0^2(\Gamma)$ of $\imath$ is the L^2-orthogonal projection onto $L_0^2(\Gamma)$. The unique solution of (1.1) is again characterized by (1.4), where the orthogonal projection now takes the form

$$\mathrm{P}_{U_{ad}}(v) = \mathrm{P}_{[a,b]}(v+m)$$

with $m \in \mathbb{R}$ chosen such that

$$\int_\Gamma \mathrm{P}_{[a,b]}(v+m)\,\mathrm{d}\Gamma = 0\,.$$

If for $v \in L^2(\Gamma)$ the inactive set $\mathcal{I}(v+m) = \{\gamma \in \Gamma \mid a < v[\gamma] + m < b\}$ is non-empty, the constant m = m(v) is uniquely determined by $v \in L^2(\Gamma)$. Hence, the solution $u \in U_{ad}$ satisfies

$$u = \mathrm{P}_{[a,b]}\left(-\frac{1}{\alpha}p(u) + m\left(-\frac{1}{\alpha}p(u)\right)\right),$$

with $p(u) = S^*(Su - \imath^* z) \in H^2(\Gamma)$ denoting the adjoint state and $m(-\frac{1}{\alpha}p(u)) \in \mathbb{R}$ is implicitly given by $\int_\Gamma u\,\mathrm{d}\Gamma = 0$. Note that $\imath^*\imath$ is the identity on $L^2_0(\Gamma)$.

In (2.2) we now replace U^h_{ad} by $U^h_{ad} = \left\{v \in L^2(\Gamma^h) \mid a \le v \le b\right\} \cap L^2_0(\Gamma^h)$. Similar as in (2.5), the unique solution u_h then satisfies

$$u_h = \mathrm{P}_{U^h_{ad}}\left(-\frac{1}{\alpha}p_h(u_h)\right) = \mathrm{P}_{[a,b]}\left(-\frac{1}{\alpha}p_h(u_h) + m_h\left(-\frac{1}{\alpha}p_h(u_h)\right)\right), \tag{4.1}$$

with $p_h(v_h) = S_h^*(S_h v_h - \imath_h^* z_l) \in H^1(\Gamma^h)$ and $m_h(-\frac{1}{\alpha}p_h(u_h)) \in \mathbb{R}$ the unique constant such that $\int_{\Gamma^h} u_h\,\mathrm{d}\Gamma^h = 0$. Note that $m_h\left(-\frac{1}{\alpha}p_h(u_h)\right)$ is semi-smooth with respect to u_h and thus Equation (4.1) is amenable to a semi-smooth Newton method.

The discretization error between the problems (2.2) and (1.1) now decomposes into two components, one introduced by the discretization of U_{ad} through the discretization of the surface, the other by discretization of S.

For the first error we need to investigate the relation between $\mathrm{P}_{U^h_{ad}}(u)$ and $\mathrm{P}_{U_{ad}}(u)$, which is now slightly more involved than in (2.6).

Lemma 4.1. *There exists a constant $C_m > 0$ depending only on Γ, $|a|$ and $|b|$ such that for all $v \in L^2(\Gamma)$ with $\int_{\mathcal{I}(v+m(v))}\mathrm{d}\Gamma > 0$ there holds*

$$|m_h(v_l) - m(v)| \le \frac{C_m}{\int_{\mathcal{I}(v+m(v))}\mathrm{d}\Gamma}h^2, \tag{4.2}$$

for $0 < h < h_v$ sufficiently small, where $h_v > 0$ depends on v.

Proof. For $v \in L^2(\Gamma)$, $\epsilon > 0$ choose $\delta > 0$ and $h > 0$ so small that the set

$$\mathcal{I}^\delta_v = \left\{\gamma \in \Gamma^h \mid a + \delta \le v_l(\gamma) + m(v) \le b - \delta\right\}, \tag{4.3}$$

satisfies

$$\int_{\mathcal{I}^\delta_v}\mathrm{d}\Gamma^h(1+\epsilon) \ge \int_{\mathcal{I}(v+m(v))}\mathrm{d}\Gamma.$$

It is easy to show that hence $m_h(v_l)$ is unique. Set $C = c_{\mathrm{int}}\max(|a|,|b|)\int_\Gamma \mathrm{d}\Gamma$. Decreasing h further if necessary ensures

$$\frac{Ch^2}{\int_{\mathcal{I}^\delta_v}\mathrm{d}\Gamma^h} \le (1+\epsilon)\frac{Ch^2}{\int_{\mathcal{I}(v+m(v))}\mathrm{d}\Gamma} \le \delta\,. \tag{4.4}$$

Because of $\int_{\mathcal{I}_v^\delta} \mathrm{d}\Gamma^h > 0$, the monotonous function $M_v^h : \mathbb{R} \to \mathbb{R}$

$$M_v^h(x) = \int_{\Gamma^h} \mathrm{P}_{[a,b]}\left(v_l + x\right) \mathrm{d}\Gamma^h\,, \tag{4.5}$$

is strictly monotonous at $m(v)$. Since $\int_\Gamma \mathrm{P}_{[a,b]}\left(v + m(v)\right) \mathrm{d}\Gamma = 0$, Lemma 2.1 yields

$$|M_v^h(m(v))| \le c_{\mathrm{int}} \|\mathrm{P}_{[a,b]}\left(v + m(v)\right)\|_{L^1(\Gamma)} h^2 \le Ch^2\,. \tag{4.6}$$

Let us assume w.l.o.g. $-Ch^2 \le M_v^h(m(v)) \le 0$. Due to (strict) monotonicity of $M_v^h(\cdot)$ this implies $m(v) \le m_h(v_l)$. Then again, since $\frac{Ch^2}{\int_{\mathcal{I}_v^\delta} \mathrm{d}\Gamma^h} \le \delta$, we conclude

$$\begin{aligned} & M_v^h\left(m(v) + \frac{Ch^2}{\int_{\mathcal{I}_v^\delta} \mathrm{d}\Gamma^h}\right) \\ & \ge M_v^h\left(m(v)\right) + \int_{\mathcal{I}_v^\delta} \frac{Ch^2}{\int_{\mathcal{I}_v^\delta} \mathrm{d}\Gamma^h} \mathrm{d}\Gamma^h = M_v^h\left(m(v)\right) + Ch^2 \ge 0\,, \end{aligned} \tag{4.7}$$

and again by strict monotonicity of $M_v^h(\cdot)$ it follows

$$m_h(v_l) \le m(v) + \frac{Ch^2}{\int_{\mathcal{I}_v^\delta} \mathrm{d}\Gamma^h}.$$

Alltogether we get

$$0 \le m_h(v_l) - m(v) \le \frac{Ch^2}{\int_{\mathcal{I}_v^\delta} \mathrm{d}\Gamma^h} \le \frac{(1+\epsilon)C}{\int_{\mathcal{I}(v+m(v))} \mathrm{d}\Gamma} h^2.$$

This proves the claim. □

Because

$$\left(\mathrm{P}_{U_{ad}^h}\left(v_l\right)\right)^l - \mathrm{P}_{U_{ad}}\left(v\right) = \mathrm{P}_{[a,b]}\left(v + m_h(v_l)\right) - \mathrm{P}_{[a,b]}\left(v + m(v)\right)\,, \tag{4.8}$$

we get the following corollary.

Corollary 4.2. *Let $v \in L^2(\Gamma)$ with $\int_{\mathcal{I}(v+m(v))} \mathrm{d}\Gamma > 0$. With C_m and $h_v > 0$ as in Lemma 4.1 there holds for $0 < h < h_v$*

$$\left\|\left(\mathrm{P}_{U_{ad}^h}\left(v_l\right)\right)^l - \mathrm{P}_{U_{ad}}\left(v\right)\right\|_{L^2(\Gamma)} \le C_m \frac{\sqrt{\int_\Gamma \mathrm{d}\Gamma}}{\int_{\mathcal{I}(v+m(v))} \mathrm{d}\Gamma} h^2\,. \tag{4.9}$$

Note that since for $u \in L^2(\Gamma)$ the adjoint $p(u)$ is a continuous function on Γ, the corollary is applicable for $v = -\frac{1}{\alpha}p(u)$.

The following theorem can be proved along the lines of Theorem 2.2.

Theorem 4.3. *Let $u \in L^2(\Gamma)$, $u_h \in L^2(\Gamma^h)$ be the solutions of (1.1) and (2.2), respectively, in the case $\mathbf{c} = 0$. Let $\tilde{u}_h = \left(\mathrm{P}_{U_{ad}^h}\left(-\frac{1}{\alpha}p(u)_l\right)\right)^l$. Then there holds for $\epsilon > 0$ and $0 \le h < h_\epsilon$*

$$\begin{aligned} & \alpha\|u_h^l - \tilde{u}_h\|_{L^2(\Gamma)}^2 + \left\|y_h^l - y\right\|_{L^2(\Gamma)}^2 \\ \le & (1+\epsilon)\left(\frac{1}{\alpha}\left\|\left((\cdot)^l S_h^*(\cdot)_l - S^*\right)(y - z)\right\|_{L^2(\Gamma)}^2 \cdots + \left\|(\cdot)^l S_h(\cdot)_l \tilde{u}_h - y\right\|_{L^2(\Gamma)}^2\right). \end{aligned}$$

Using Corollary 4.2 we conclude from the theorem

$$\begin{aligned}
&\|u_h^l - u\|_{L^2(\Gamma)} \\
&\leq C\left(\frac{1}{\alpha}\left\|\left((\cdot)^l S_h^*(\cdot)_l - S^*\right)(y-z)\right\|_{L^2(\Gamma)} + \frac{1}{\sqrt{\alpha}}\left\|\left((\cdot)^l S_h(\cdot)_l - S\right)u\right\|_{L^2(\Gamma)}\cdots\right. \\
&\left.\quad + \left(1 + \frac{\|S\|_{\mathcal{L}(L^2(\Gamma),L^2(\Gamma))}}{\sqrt{\alpha}}\right)\frac{C_m\sqrt{\int_\Gamma \mathrm{d}\Gamma}\, h^2}{\int_{\mathcal{I}(-\frac{1}{\alpha}p(u)+m(-\frac{1}{\alpha}p(u)))}\mathrm{d}\Gamma}\right), \qquad (4.10)
\end{aligned}$$

the latter part of which is the error introduced by the discretization of U_{ad}. Hence one has h^2-convergence of the optimal controls.

Eq.(4.1) is amenable to a semi-smooth Newton method as described in Section 3. The algorithm however needs to take the scalar quantity $m_h\left(-\frac{1}{\alpha}p_h(v)\right)$ into account for each iterate $v \in L^2(\Gamma^h)$. The functional $m_h\left(-\frac{1}{\alpha}p_h(\cdot)\right)$ can be shown to be semi-smooth with generalized derivative $\frac{-1}{\int_{\Gamma^h}\chi\,\mathrm{d}\Gamma^h}\int_{\Gamma^h}\frac{\chi}{\alpha}S_h^*S_h\,\mathrm{d}\Gamma^h$ and is evaluated by performing a Newton algorithm on

$$\int_{\Gamma^h} \mathrm{P}_{[a,b]}\left(-\frac{1}{\alpha}p_h(v) + m_h\right)\mathrm{d}\Gamma^h = 0\,. \qquad (4.11)$$

5. Numerical Examples

The figures show some selected Newton steps u^+. Note that jumps of the color-coded function values are well observable along the border between active and inactive set. For all examples Newton's method is initialized with $u_0 \equiv 0$.

The meshes are generated from a macro triangulation through congruent refinement, new nodes are projected onto the surface Γ. The maximal edge length h in the triangulation is not exactly halved in each refinement, but up to an error of order $O(h^2)$. Therefore we just compute our estimated order of convergence (EOC) according to

$$EOC_i = \frac{\ln\|u_{h_{i-1}} - u_l\|_{L^2(\Gamma^{h_{i-1}})} - \ln\|u_{h_i} - u_l\|_{L^2(\Gamma^{h_i})}}{\ln(2)}.$$

For different refinement levels, the tables show L^2-errors, the corresponding EOC and the number of Newton iterations before the desired accuracy of 10^{-6} is reached.

It was shown in [8], under certain assumptions on the behaviour of $-\frac{1}{\alpha}p(u)$, that the undamped Newton Iteration is mesh-independent. These assumptions are met by all our examples, since the surface gradient of $-\frac{1}{\alpha}p(u)$ is bounded away from zero along the border of the inactive set. Moreover, the displayed number of Newton-Iterations suggests mesh-independence of the semi-smooth Newton method.

Example 5.1 (Sphere I) *We consider the problem*

$$\min_{u\in L^2(\Gamma),\, y\in H^1(\Gamma)} J(u,y)$$
$$\textit{subject to} \quad -\Delta_\Gamma y + y = u - r, \quad -1 \leq u \leq 1 \qquad (5.1)$$

with Γ *the unit sphere in* $\mathbb{R}^3$ *and* $\alpha = 1.5\cdot 10^{-6}$. *We choose* $z = 52\alpha x_3(x_1^2 - x_2^2)$ *, to obtain the solution*

$$\bar{u} = r = \min\left(1, \max\left(-1, 4x_3(x_1^2 - x_2^2)\right)\right)$$

of (5.1).

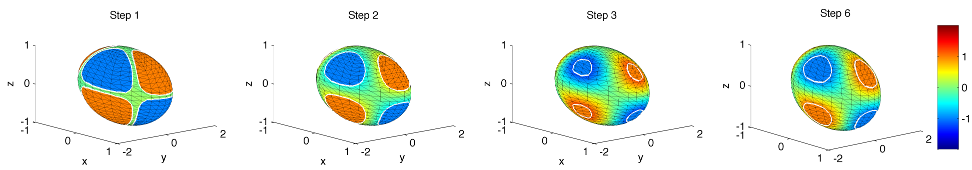

Fig. 5.1. Selected full Steps u^+ computed for Example 5.1 on the twice refined sphere.

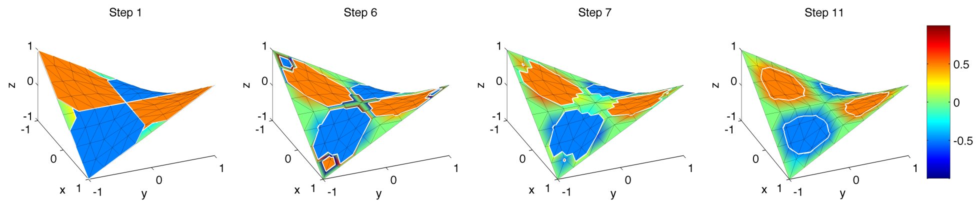

Fig. 5.2. Selected full Steps u^+ computed for Example 5.2 on the twice refined grid.

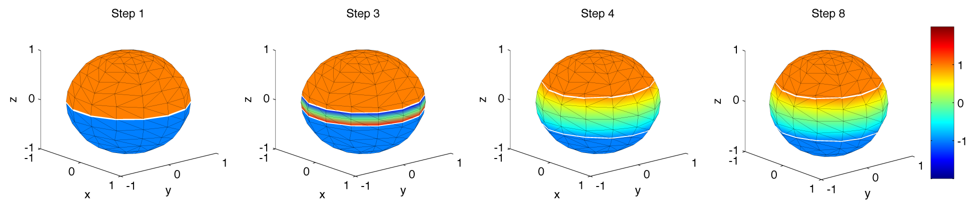

Fig. 5.3. Selected full Steps u^+ computed for Example 5.3 on once refined sphere.

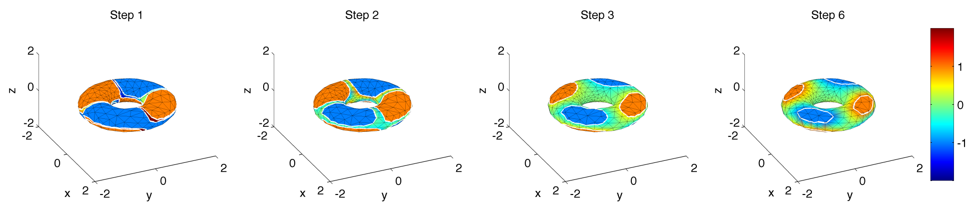

Fig. 5.4. Selected full Steps u^+ computed for Example 5.4 on the once refined torus.

Example 5.2. *Let* $\Gamma = \big\{(x_1, x_2, x_3)^T \in \mathbb{R}^3 \mid x_3 = x_1 x_2 \wedge x_1, x_2 \in (0,1)\big\}$ *and* $\alpha = 10^{-3}$. *For*

$$\min_{u\in L^2(\Gamma),\, y\in H^1(\Gamma)} J(u,y)$$

$$\text{subject to } -\Delta_\Gamma y = u - r, \quad y = 0 \text{ on } \partial\Gamma \quad -0.5 \le u \le 0.5$$

we get

$$\bar{u} = r = \max\big(-0.5, \min\big(0.5, \sin(\pi x)\sin(\pi y)\big)\big)$$

by proper choice of z *(via symbolic differentiation).*

Example 5.2, although $\mathbf{c} = 0$, is also covered by the theory in Sections 1-3, as by the Dirichlet boundary conditions the state equation remains uniquely solvable for $u \in L^2(\Gamma)$. In the last two examples we apply the variational discretization to optimization problems, that involve zero-mean-value constraints as in Section 4.

Example 5.3 (Sphere II) *We consider*

$$\min_{u\in L^2(\Gamma),\, y\in H^1(\Gamma)} J(u,y)$$

$$\text{subject to } -\Delta_\Gamma y = u\,, \quad -1 \le u \le 1\,, \quad \int_\Gamma y\,\mathrm{d}\Gamma = \int_\Gamma u\,\mathrm{d}\Gamma = 0\,,$$

with Γ *the unit sphere in* $\mathbb{R}^3$. *Set* $\alpha = 10^{-3}$ *and*

$$z(x_1,x_2,x_3) = 4\alpha x_3 + \begin{cases} \ln(x_3+1)+C\,, & \text{if} \quad 0.5 \le x_3 \\ x_3 - \frac{1}{4}\operatorname{arctanh}(x_3)\,, & \text{if} \quad -0.5 \le x_3 \le 0.5 \\ -C - \ln(1-x_3)\,, & \text{if} \quad x_3 \le -0.5 \end{cases}\,,$$

where C *is chosen for* z *to be continuous. The solution according to these parameters is*

$$\bar{u} = \min\big(1, \max\big(-1, 2x_3\big)\big)\,.$$

Example 5.4 (Torus) *Let* $\alpha = 10^{-3}$ *and*

$$\Gamma = \left\{ (x_1,x_2,x_3)^T \in \mathbb{R}^3 \;\middle|\; \sqrt{x_3^2 + \left(\sqrt{x_1^2+x_2^2}-1\right)^2} = \frac{1}{2} \right\}$$

Table 5.1: L^2-error, EOC and number of iterations for Example 5.1.

reg. refs.	0	1	2	3	4	5
$L2$-error	5.8925e-01	1.4299e-01	3.5120e-02	8.7123e-03	2.2057e-03	5.4855e-04
EOC	-	2.0430	2.0255	2.0112	1.9818	2.0075
# Steps	6	6	6	6	6	6

Table 5.2: L^2-error, EOC and number of iterations for Example 5.2.

reg. refs.	0	1	2	3	4	5
$L2$-error	3.5319e-01	6.6120e-02	1.5904e-02	3.6357e-03	8.8597e-04	2.1769e-04
EOC	-	2.4173	2.0557	2.1291	2.0369	2.0250
# Steps	11	12	12	11	13	12

Table 5.3: L^2-error, EOC and number of iterations for Example 5.3.

reg. refs.	0	1	2	3	4	5
$L2$-error	6.7223e-01	1.6646e-01	4.3348e-02	1.1083e-02	2.7879e-03	6.9832e-04
EOC	-	2.0138	1.9412	1.9677	1.9911	1.9972
# Steps	8	8	7	7	6	6

Table 5.4: L^2-error, EOC and number of iterations for Example 5.4.

reg. refs.	0	1	2	3	4	5
$L2$-error	3.4603e-01	9.8016e-02	2.6178e-02	6.6283e-03	1.6680e-03	4.1889e-04
EOC	-	1.8198e+00	1.9047e+00	1.9816e+00	1.9905e+00	1.9935e+00
# Steps	9	3	3	3	2	2

the 2-Torus embedded in $\mathbb{R}^3$*. By symbolic differentiation we compute z, such that*

$$\min_{u\in L^2(\Gamma),\, y\in H^1(\Gamma)} J(u,y)$$
$$\textit{subject to } -\Delta_\Gamma y = u - r, \quad -1 \le u \le 1\,, \quad \int_\Gamma y\,\mathrm{d}\Gamma = \int_\Gamma u\,\mathrm{d}\Gamma = 0$$

is solved by

$$\bar{u} = r = \max\big(-1, \min\big(1, 5xyz\big)\big)\,.$$

As the presented tables clearly demonstrate, the examples show the expected convergence behaviour.

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