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operator on compact surfaces - concept
and numerical treatment**

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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.

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1 Introduction

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

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

with $U_{ad} = \{v \in L^2(\Gamma) \mid a \leq v \leq b\}$, $a < b \in \mathbb{R}$. 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 .

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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 [Hin05] and [HPUU09], on a discrete surface Γ^h approximating Γ . The discretization of the state equation in (1.1) is achieved by the finite element method proposed in [Dzi88], 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 [Dem09], and steps towards a posteriori error control for elliptic PDEs on surfaces are taken by Demlow and Dziuk in [DD07]. For alternative approaches for the discretization of the state equation by finite elements see the work of Burger [Bur08]. Finite element methods on moving surfaces are developed by Dziuk and Elliott in [DE07]. 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 with unit normal field ν . As an embedded, compact hypersurface in \mathbb{R}^{n+1} it is orientable and hence the zero level set of a signed distance function $|d(x)| = \text{dist}(x, \Gamma)$. We assume w.l.o.g. $\nabla d(x) = \nu(x)$ for $x \in \Gamma$. Further, there exists a 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

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

is unique, see e.g. [GT98, Lemma 14.16]. Note that $\nabla d(x) = \nu(a(x))$.

Using a we can extend any function $\phi : \Gamma \rightarrow \mathbb{R}$ 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. $\Delta_{\Gamma} : H^1(\Gamma) \rightarrow H^1(\Gamma)^*$

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

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

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

which is compact and constitutes a linear homeomorphism onto $H^2(\Gamma)$, see [Dzi88, 1. Theorem].

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

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

We rewrite (1.3) as

$$u = P_{U_{ad}} \left(-\frac{1}{\alpha} S^*(Su - z) \right), \quad (1.4)$$

where $P_{U_{ad}}$ 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 $(\cdot)_l : L^2(\Gamma) \rightarrow L^2(\Gamma^h)$ defines a linear homeomorphism with inverse $(\cdot)^l$. Moreover, there exists $c_{\text{int}} > 0$ such that

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

as the following lemma shows.

Lemma and Definition 2.1. Denote by $\frac{d\Gamma}{d\Gamma^h}$ the Jacobian of $a|_{\Gamma^h} : \Gamma^h \rightarrow \Gamma$, i.e. $\frac{d\Gamma}{d\Gamma^h} = |\det(M)|$ where $M \in \mathbb{R}^{n \times n}$ represents the Derivative $da(x) : T_x \Gamma^h \rightarrow T_{a(x)} \Gamma$ with respect to arbitrary orthonormal bases of the respective tangential space. For small $h > 0$ there holds

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

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

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

Proof. see [DE07, Lemma 5.1] ■

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

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

with $U_{ad}^h = \{v \in L^2(\Gamma^h) \mid a \leq v \leq b\}$, 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 [Hin05] to optimal control problems on surfaces.

In [Dzi88] it is explained, how to implement a discrete solution operator $S_h : L^2(\Gamma^h) \rightarrow L^2(\Gamma^h)$, such that

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

which we will use throughout this paper. See in partikular [Dzi88, Equation (6)] and [Dzi88, 7. Lemma]. For the convenience of the reader we briefly sketch the method. Consider the space

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

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

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

for $y_h \in V_h$. We choose $L^2(\Gamma^h)$ as control space, because in general we cannot evaluate $\int_{\Gamma} v \, d\Gamma$ exactly, whereas the expression $\int_{\Gamma^h} v_l \, d\Gamma^h$ 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

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

hence evaluating $(\cdot)_l^*$ and $(\cdot)^{l*}$ requires knowledge of the Jacobians $\frac{d\Gamma^h}{d\Gamma}$ and $\frac{d\Gamma}{d\Gamma^h}$ 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

$$u_h = P_{U_{ad}^h} \left(-\frac{1}{\alpha} p_h(u_h) \right). \quad (2.5)$$

Here $P_{U_{ad}^h} : L^2(\Gamma^h) \rightarrow U_{ad}^h$ 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 $P_{U_{ad}}$ and $P_{U_{ad}^h}$ coincide with the point-wise projection $P_{[a,b]}$ on Γ and Γ^h , respectively, and hence

$$\left(P_{U_{ad}^h}(v_l) \right)^l = P_{U_{ad}}(v) \quad (2.6)$$

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*

$$\alpha \|u_h^l - u\|_{L^2(\Gamma)}^2 + \|y_h^l - y\|_{L^2(\Gamma)}^2 \leq \frac{1 + c_{\text{int}} h^2}{1 - c_{\text{int}} h^2} \left(\frac{1}{\alpha} \left\| \left((\cdot)^l S_h^*(\cdot)_l - S^* \right) (y - z) \right\|_{L^2(\Gamma)}^2 \dots \right. \\ \left. + \left\| \left((\cdot)^l S_h(\cdot)_l - S \right) u \right\|_{L^2(\Gamma)}^2 \right), \quad (2.7)$$

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

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

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

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

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

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

Adding these inequalities yields

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

The first addend is estimated via

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

The second addend satisfies

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

Together this yields

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

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

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

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

$$\|((\cdot)_l)^* - (\cdot)^l\|_{\mathcal{L}(L^2(\Gamma^h), L^2(\Gamma))} \leq c_{\text{int}} h^2, \quad \|((\cdot)^l)^* - (\cdot)_l\|_{\mathcal{L}(L^2(\Gamma), L^2(\Gamma^h))} \leq c_{\text{int}} h^2. \quad (2.9)$$

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

3 Implementation

In order to solve (2.5) numerically, we proceed as in [Hin05] using the finite element techniques for PDEs on surfaces developed in [Dzi88] combined with the semi-smooth Newton techniques from [HIK03] and [Ul03] applied to the equation

$$G_h(u_h) = \left(u_h - P_{[a,b]} \left(-\frac{1}{\alpha} p_h(u_h) \right) \cdot \right) = 0 \quad (3.1)$$

Since the operator p_h continuously maps $v \in L^2(\Gamma^h)$ into $H^1(\Gamma^h)$, Equation (3.1) is semi-smooth 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 $\chi : \Gamma^h \rightarrow \{0, 1\}$ denotes the indicator function of the inactive set $\mathcal{I}(-\frac{1}{\alpha}p_h(u)) = \{\gamma \in \Gamma^h \mid a < -\frac{1}{\alpha}p_h(u)[\gamma] < b\}$

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

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

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

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

1. Set $((1 - \chi)u^+)[\gamma] = ((1 - \chi)P_{[a,b]}(-\frac{1}{\alpha}p_h(u) + m))[\gamma]$, 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 [HV11].

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

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

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

Using the injection $L_0^2(\Gamma) \xrightarrow{\iota} L^2(\Gamma)$, \tilde{S} is prolonged as an operator $S : L^2(\Gamma) \rightarrow L^2(\Gamma)$ by $S = \iota\tilde{S}\iota^*$. The adjoint $\iota^* : L^2(\Gamma) \rightarrow L_0^2(\Gamma)$ of ι 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

$$P_{U_{ad}}(v) = P_{[a,b]}(v + m)$$

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

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

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

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

with $p(u) = S^*(Su - i^*z) \in H^2(\Gamma)$ denoting the adjoint state and $m(-\frac{1}{\alpha}p(u)) \in \mathbb{R}$ is implicitly given by $\int_{\Gamma} u \, d\Gamma = 0$. Note that i^*i is the identity on $L_0^2(\Gamma)$.

In (2.2) we now replace U_{ad}^h by $U_{ad}^h = \{v \in L^2(\Gamma^h) \mid a \leq v \leq b\} \cap L_0^2(\Gamma^h)$. Similar as in (2.5), the unique solution u_h then satisfies

$$u_h = P_{U_{ad}^h} \left(-\frac{1}{\alpha} p_h(u_h) \right) = P_{[a,b]} \left(-\frac{1}{\alpha} p_h(u_h) + m_h \left(-\frac{1}{\alpha} p_h(u_h) \right) \right), \quad (4.1)$$

with $p_h(v_h) = S_h^*(S_h v_h - i_h^* z_l) \in H^1(\Gamma^h)$ and $m_h(-\frac{1}{\alpha}p_h(u_h)) \in \mathbb{R}$ the unique constant such that $\int_{\Gamma^h} u_h \, d\Gamma^h = 0$. Note that $m_h(-\frac{1}{\alpha}p_h(u_h))$ 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 $P_{U_{ad}^h}(u)$ and $P_{U_{ad}}(u)$, which is now slightly more involved than in (2.6).

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

$$|m_h(v_l) - m(v)| \leq \frac{C_m}{\int_{\mathcal{I}(v+m(v))} d\Gamma} h^2.$$

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

$$\mathcal{I}_v^\delta = \left\{ \gamma \in \Gamma^h \mid a + \delta \leq v_l(\gamma) + m(v) \leq b - \delta \right\}.$$

satisfies $\int_{\mathcal{I}_v^\delta} d\Gamma^h (1 + \epsilon) \geq \int_{\mathcal{I}(v+m(v))} d\Gamma$. It is easy to show that hence $m_h(v_l)$ is unique. Set $C = c_{\text{int}} \max(|a|, |b|) \int_{\Gamma} d\Gamma$. Decreasing h further if necessary ensures

$$\frac{Ch^2}{\int_{\mathcal{I}_v^\delta} d\Gamma^h} \leq (1 + \epsilon) \frac{Ch^2}{\int_{\mathcal{I}(v+m(v))} d\Gamma} \leq \delta.$$

For $x \in \mathbb{R}$ let

$$M_v^h(x) = \int_{\Gamma^h} P_{[a,b]}(v_l + x) \, d\Gamma^h.$$

Since $\int_{\Gamma} P_{[a,b]}(v + m(v)) \, d\Gamma = 0$, Lemma 2.1 yields

$$|M_v^h(m(v))| \leq c_{\text{int}} \|P_{[a,b]}(v + m(v))\|_{L^1(\Gamma)} h^2 \leq Ch^2.$$

Let us assume w.l.o.g. $-Ch^2 \leq M_v^h(m(v)) \leq 0$. Then

$$M_v^h \left(m(v) + \frac{Ch^2}{\int_{\mathcal{I}_v^\delta} d\Gamma^h} \right) \geq M_v^h(m(v)) + Ch^2 \geq 0$$

implies $0 \leq m(v) - m_h(v) \leq \frac{Ch^2}{\int_{\mathcal{I}_v^{\delta}} d\Gamma^h} \leq \frac{(1+\epsilon)C}{\int_{\mathcal{I}(v+m(v))} d\Gamma} h^2$, since $M_v^h(x)$ is continuous with respect to x . This proves the claim. \blacksquare

Because

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

we get the following corollary.

Corollary 4.2. *Let $h > 0$ be sufficiently small and C_m as in Lemma 4.1. For any fixed $v \in L^2(\Gamma)$ with $\int_{\mathcal{I}(v+m(v))} d\Gamma > 0$ we have*

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

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 proofed 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 $\tilde{u}_h = \left(\mathbb{P}_{U_{ad}^h} \left(-\frac{1}{\alpha}p(u_l) \right) \right)^l$. Then there holds for $\epsilon > 0$ and $0 \leq h < h_\epsilon$*

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

Using Corollary 4.2 we conclude from the theorem

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

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.

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

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

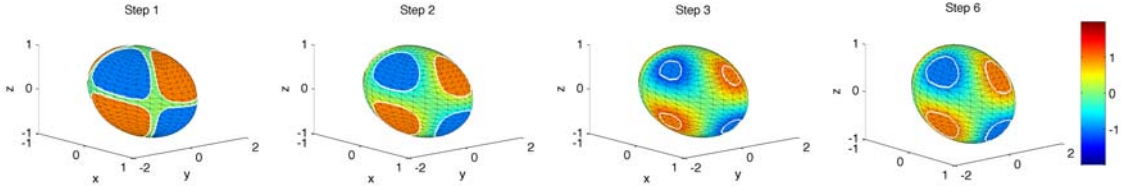


Figure 1: Selected full Steps u^+ computed for Example 5.1 on the twice refined sphere.

reg. refs.	0	1	2	3	4	5
L^2 -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 1: L^2 -error, EOC and number of iterations for Example 5.1.

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 [HU04], under certain assumptions on the behaviour of $-\frac{1}{\alpha}p(u)$, that the undamped Newton Iteration is mesh-intdependent. 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

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

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

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

of (5.1).

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

$$\min_{u \in L^2(\Gamma), y \in H^1(\Gamma)} J(u, y) \text{ subject to } -\Delta_{\Gamma} y = u - r, \quad y = 0 \text{ on } \partial\Gamma \quad -0.5 \leq u \leq 0.5$$

we get

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

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.

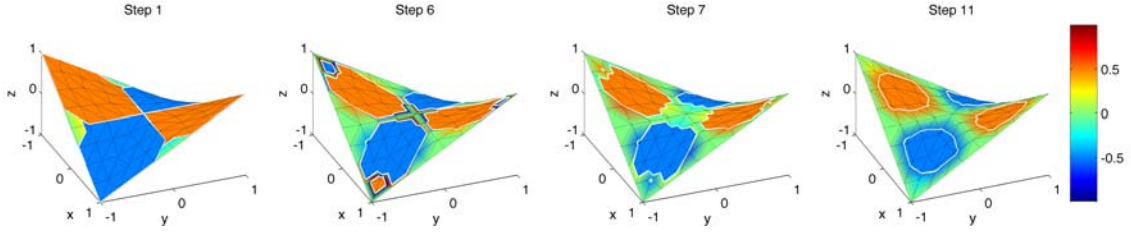


Figure 2: Selected full Steps u^+ computed for Example 5.2 on the twice refined grid.

reg. refs.	0	1	2	3	4	5
L^2 -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 2: L^2 -error, EOC and number of iterations for Example 5.2.

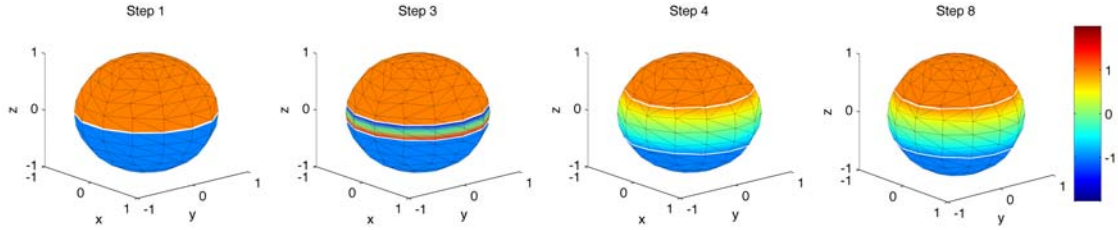


Figure 3: Selected full Steps u^+ computed for Example 5.3 on once refined sphere.

reg. refs.	0	1	2	3	4	5
L^2 -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 3: L^2 -error, EOC and number of iterations for Example 5.3.

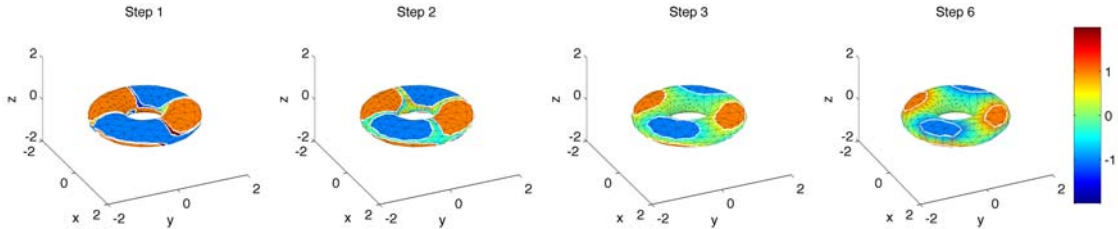


Figure 4: Selected full Steps u^+ computed for Example 5.4 on the once refined torus.

reg. refs.	0	1	2	3	4	5
L^2 -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

Table 4: L^2 -error, EOC and number of iterations for Example 5.4.

Example 5.3 (Sphere II). We consider

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

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

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

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

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

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

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

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

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

is solved by

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

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

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