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 \( \Gamma \subset \mathbb{R}^{n+1} \), \( n = 1, 2 \).

\[
\begin{aligned}
\min_{u \in L^2(\Gamma), y \in H^1(\Gamma)} & \quad J(u, y) = \frac{1}{2} \| y - z \|_{L^2(\Gamma)}^2 + \frac{\alpha}{2} \| u \|_{L^2(\Gamma)}^2 \\
\text{subject to} & \quad u \in U_{ad} \quad \text{and} \\
& \quad \int_{\Gamma} \nabla y \nabla \phi + cy \phi \, d\Gamma = \int_{\Gamma} u \phi \, d\Gamma, \forall \phi \in H^1(\Gamma)
\end{aligned}
\]

(1.1)

with \( U_{ad} = \{ v \in L^2(\Gamma) \mid a \leq v \leq b \} \), \( a < b \in \mathbb{R} \). For simplicity we will assume \( \Gamma \) to be compact and \( c = 1 \). In section 4 we briefly investigate the case \( c = 0 \), 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 \( \Gamma \) 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 \( \Gamma^h \) approximating \( \Gamma \). 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 \( \Gamma \) is of class \( C^2 \) with unit normal field \( \nu \). 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 an neighborhood \( N \subset \mathbb{R}^{n+1} \) of \( \Gamma \), such that \( d \) is also of class \( C^2 \) on \( N \) and the projection

\begin{equation}
    a : N \rightarrow \Gamma, \quad a(x) = x - d(x)\nabla d(x) \tag{1.2}
\end{equation}

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 \( N \) as \( \hat{\phi}(x) = \phi(a(x)) \). This allows us to represent the surface gradient in global exterior coordinates \( \nabla_{\Gamma} \phi = (I - \nu \nu^T) \nabla \hat{\phi} \), with the euclidean projection \((I - \nu \nu^T)\) onto the tangential space of \( \Gamma \).

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 prolongated restricted solution operator of the state equation

\[ S : L^2(\Gamma) \rightarrow L^2(\Gamma), \quad u \mapsto y - \Delta_{\Gamma} y + cy = u, \]

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 \( u \in U_{ad} \)

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

We rewrite (1.3) as

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

where \( P_{U_{ad}} \) denotes the \( L^2 \)-orthogonal projection onto \( U_{ad} \).

2 Discretization

We now discretize (1.1) using an approximation \( \Gamma^h \) to \( \Gamma \) which is globally of class \( C^{0,1} \).

Following Dziuk, we consider polyhedral \( \Gamma^h = \bigcup_{i \in I_h} T^i_h \) consisting of triangles \( T^i_h \) with corners
on \( \Gamma \), whose maximum diameter is denoted by \( h \). With FEM error bounds in mind we assume the family of triangulations \( \Gamma^h \) to be regular in the usual sense that the angles of all triangles are bounded away from zero uniformly in \( h \).

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

\[
y'(a(x)) = y(x) \quad \forall x \in \Gamma^h,
\]

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

\[
y_h(x) = y(a(x)) \quad \forall x \in \Gamma^h.
\]

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

\[
1 - c_{\text{int}} h^2 \leq \| (\cdot)_l \|_{L^2(\Gamma^h),L^2(\Gamma^h)}^2, \quad \| (\cdot)'_l \|_{L^2(\Gamma^h),L^2(\Gamma)}^2 \leq 1 + c_{\text{int}} h^2, \tag{2.1}
\]

as the following lemma shows.

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

\[
\sup_{\Gamma^h} \left| 1 - \frac{\partial}{\partial \Gamma^h} \right| \leq c_{\text{int}} h^2,
\]

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

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

**Proof.** see [DE07, Lemma 5.1]

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

\[
\min_{u \in L^2(\Gamma^h), y \in H^1(\Gamma^h)} J(u, y) = \frac{1}{2} \| y - z_l \|_{L^2(\Gamma^h)}^2 + \frac{\alpha}{2} \| u \|_{L^2(\Gamma^h)}^2 \tag{2.2}
\]

subject to \( u \in U_{\text{ad}}^h \) and \( y = S_h u \),

with \( U_{\text{ad}}^h = \{ v \in L^2(\Gamma^h) \mid a \leq v \leq b \} \), i.e. the mesh parameter \( h \) enters into \( U_{\text{ad}} \) only through \( \Gamma^h \). 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 \( S_h : L^2(\Gamma^h) \to L^2(\Gamma^h) \), such that

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

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

\[
V_h = \left\{ \varphi \in C^0(\Gamma^h) \mid \forall i \in I_h : \varphi|_{T_{ih}} \in \mathcal{P}^1(T_{ih}) \right\} \subset H^1(\Gamma^h)
\]
of piecewise linear, globally continuous functions on $\Gamma^h$. For some $u \in L^2(\Gamma)$, to compute $y_h^l = (\cdot)^t P_h (\cdot) u$ solve

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

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

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

(2.4)
hence evaluating $(\cdot)^* t$ and $(\cdot)^t$ 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 $u_h \in U^h_{ad}$ which satisfies

$$
u_h = P^{u^h}_{U^h_{ad}} \left( - \frac{1}{\alpha} p_h (u_h) \right).
$$

(2.5)

Here $P^{u^h}_{U^h_{ad}} : L^2(\Gamma^h) \to U^h_{ad}$ is the $L^2(\Gamma^h)$-orthogonal projection onto $U^h_{ad}$ 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 $P^{u^h}_{U^h_{ad}}$ coincide with the point-wise projection $P_{[a,b]}$ on $\Gamma$ and $\Gamma^h$, respectively, and hence

$$
(P^{u^h}_{U^h_{ad}} (v_l))^t = P_{U_{ad}} (v)
$$

(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

$$
\alpha \| u_h - u \|^2_{L^2(\Gamma)} + \| y_h^l - y \|^2_{L^2(\Gamma)} \leq \frac{1}{1 - c_{int} h^2} \left( \frac{1}{\alpha} \left( \| (\cdot)^t S_h (\cdot)^t - S^* \right) (y - z) \right)^2_{L^2(\Gamma)} \ldots
$$

$$
+ \left( \| (\cdot)^t S_h (\cdot)^t - S \right) u \|^2_{L^2(\Gamma)},
$$

(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 $U^h_{ad}$ is $u_l$

$$
u_l = P^{u^h}_{U^h_{ad}} \left( - \frac{1}{\alpha} p_h (u_h) \right),
$$

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

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

Adding these inequalities yields

\[
\alpha\|u_l - u_h\|_{L^2(\Gamma^h)}^2 \leq \langle (p_h(u_h) - p(u)_l), u_l - u_h \rangle_{L^2(\Gamma^h)}
\]

\[
= \langle p_h(u_h) - S_h^*(y - z)_l, u_l - u_h \rangle_{L^2(\Gamma^h)} + \langle S_h^*(y - z)_l - p(u)_l, u_l - u_h \rangle_{L^2(\Gamma^h)}.
\]

The first addend is estimated via

\[
\langle p_h(u_h) - S_h^*(y - z)_l, u_l - u_h \rangle_{L^2(\Gamma^h)} = \langle y_h - y_l, S_h u_l - y_h \rangle_{L^2(\Gamma^h)}
\]

\[
= -\|y_h - y_l\|_{L^2(\Gamma^h)}^2 + \langle y_h - y_l, S_h u_l - y_l \rangle_{L^2(\Gamma^h)}
\]

\[
\leq -\frac{1}{2}\|y_h - y_l\|_{L^2(\Gamma^h)}^2 + \frac{1}{2}\|S_h u_l - y_l\|_{L^2(\Gamma^h)}^2.
\]

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

\[
\|((\cdot))^*S_h((\cdot))^* - S^*\|_{L^2(\Gamma),L^2(\Gamma)} \leq C_{FE}h^2.
\]

(2.8)

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

\[
\|((\cdot))^* - (\cdot)^l\|_{L^2(\Gamma),L^2(\Gamma)} \leq c_{int}h^2, \quad \|((\cdot))^* - (\cdot)^l\|_{L^2(\Gamma),L^2(\Gamma)} \leq c_{int}h^2.
\]

(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 [Ulb03] applied to the equation

\[
G_h(u_h) = \left( u_h - P_{[u,b]} \left( -\frac{1}{\alpha}p_h(u_h) \right) \right) = 0.
\]

(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

\[
DG_h(u) = \left( I + \frac{\lambda}{\alpha}S_h^*S_h \right),
\]
where \( \chi : \Gamma^h \to \{0, 1\} \) denotes the indicator function of the inactive set \( \mathcal{I}(-\frac{1}{\alpha}p_h(u)) = \{ \gamma \in \Gamma^h \mid a < -\frac{1}{\alpha}p_h(u)[\gamma] < b \} \):

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

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

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

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

\[
(I + \chi \alpha S^* S_h) \chi u^+ = \chi \alpha (S^* z_l - S^* S_h (1 - \chi) u^+)
\]

for \( \chi u^+ \) 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 \( c = 0 \)

In this section we investigate the case \( c = 0 \) which corresponds to a stationary, purely diffusion driven process. Since \( \Gamma \) 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

\[
U_{ad} = \{ v \in L^2(\Gamma) \mid a \leq v \leq b \} \cap L^2_0(\Gamma), \text{ where } L^2_0(\Gamma) := \{ v \in L^2(\Gamma) \mid \int_{\Gamma} v \, d\Gamma = 0 \},
\]

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 \( y = Su \) with the solution operator \( S : L^2_0(\Gamma) \to L^2_0(\Gamma) \) of the equation \(-\Delta y = u, \int_{\Gamma} y \, d\Gamma = 0 \).

Using the injection \( L^2_0(\Gamma) \hookrightarrow L^2(\Gamma) \), \( S \) is prolonged as an operator \( S : L^2(\Gamma) \to L^2(\Gamma) \) by \( S = iS \). The adjoint \( i^* : L^2(\Gamma) \to L^2_0(\Gamma) \) of \( i \) is the \( L^2 \)-orthogonal projection onto \( L^2_0(\Gamma) \). 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 $p(u) = S^* (Su - v^* z) \in H^2(\Gamma)$ 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 $v^*$ is the identity on $L_0^2(\Gamma)$.

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

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

with $p_h(v_h) = S_h^*(S_h v_h - v_h^* z_l) \in H^1(\Gamma^h)$ 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 $P_{U_{ad}^{h_a}}(u)$ 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 $\Gamma$, $|a|$ and $|b|$ such that for all $v \in L^2(\Gamma)$ with $\int_{\mathcal{I}(v+m(v))} \mathrm{d}\Gamma > 0$ there holds

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

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

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

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

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

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

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

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

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

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

$$M_h^v \left( m(v) + \frac{Ch^2}{\int_{\mathcal{I}_v^h} \mathrm{d}\Gamma^h} \right) \geq M_h^v (m(v)) + Ch^2 \geq 0.$$
implies $0 \leq m(v) - m_h(v) \leq C h^2 \int_{Z^+} \dd x \leq \frac{(1+e)C}{\int_{I^{(c+m(v))}} \dd x} h^2$, since $M_h(x)$ is continuous with respect to $x$. This proves the claim.

Because

$$\left( P_{U_{ad}}(v_i) \right)^{l} - P_{U_{ad}}(v) = P_{[a,b]}(v + m_h(v)) - P_{[a,b]}(v + m(v)),$$

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 $\int_{I(v+m(v))} \dd \Gamma > 0$ we have

$$\left\| \left( P_{U_{ad}}(v_i) \right)^{l} - P_{U_{ad}}(v) \right\|_{L^2(\Gamma)} \leq C_m \sqrt{\frac{\int_{I^{(c+m(v))}} \dd \Gamma}{\int_{I^{(c+m(v))}} \dd \Gamma}} h^2.$$ 

Note that since for $u \in L^2(\Gamma)$ the adjoint $p(u)$ is a continuous function on $\Gamma$, 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 $c = 0$. Let $\hat{u}_h = \left( P_{U_{ad}}(\frac{1}{\alpha} p(u)) \right)^{1}$. Then there holds for $\epsilon > 0$ and $0 \leq h < h_c$

$$\alpha \| u_h^l - \hat{u}_h \|_{L^2(\Gamma)} \leq \sqrt{\frac{\int_{I^{(c+m(v))}} \dd \Gamma}{\int_{I^{(c+m(v))}} \dd \Gamma}} h^2.$$ 

Using Corollary 4.2 we conclude from the theorem

$$\| u_h^l - u \|_{L^2(\Gamma)} \leq \left( \frac{1}{\alpha} \| \left( \cdot \right)^{1} S_h^l (\cdot) - S^l \|_{L^2(\Gamma)} \right) \| u - \hat{u}_h \|_{L^2(\Gamma)} + \frac{1}{\sqrt{\alpha}} \| \left( \cdot \right)^{1} S_h (\cdot) - S \|_{L^2(\Gamma)} \| u \|_{L^2(\Gamma)} \leq \frac{C_m \sqrt{\int_{I} \dd \Gamma} h^2}{\sqrt{\alpha}} \left( \frac{1 + \| S \|_{L^2(\Gamma),L^2(\Gamma)}}{\sqrt{\alpha}} \right) \left( \frac{1 + \| S \|_{L^2(\Gamma),L^2(\Gamma)}}{\sqrt{\alpha}} \right)$$

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 $\Gamma$. 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

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

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

with \( \Gamma \) 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 \( \Gamma = \{(x_1, x_2, x_3)^T \in \mathbb{R}^3 \mid x_3 = x_1x_2 \land x_1, x_2 \in (0, 1)\} \) and \( \alpha = 10^{-3} \). For

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

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 \( c = 0 \), 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.
Example 5.3 (Sphere II). We consider
\[
\min_{u \in L^2(\Gamma), y \in H^1(\Gamma)} J(u, y) \quad \text{subject to} \quad -\Delta \Gamma y = u, \quad -1 \leq u \leq 1, \quad \int_{\Gamma} y \, d\Gamma = \int_{\Gamma} u \, d\Gamma = 0,
\]
with \(\Gamma\) the unit sphere in \(\mathbb{R}^3\). Set \(\alpha = 10^{-3}\) and
\[
z(x_1, x_2, x_3) = 4\alpha x_3 + \begin{cases} 
\ln(x_3 + 1) + C, & \text{if } 0.5 \leq x_3 \\
x_3 - \frac{1}{4} \arctanh(x_3), & \text{if } -0.5 \leq x_3 \leq 0.5 \\
-C - \ln(1 - x_3), & \text{if } x_3 \leq -0.5
\end{cases}
\]
where \(C\) is chosen for \(z\) to be continuous. The solution according to these parameters is
\[
\bar{u} = \min \left( 1, \max \left( -1, 2x_3 \right) \right).
\]

Example 5.4 (Torus). Let \(\alpha = 10^{-3}\) and
\[
\Gamma = \left\{ (x_1, x_2, x_3)^T \in \mathbb{R}^3 \left| \sqrt{x_1^2 + \left( \sqrt{x_1^2 + x_2^2} - 1 \right)^2} = \frac{1}{2} \right. \right\}
\]
the 2-Torus embedded in \(\mathbb{R}^3\). By symbolic differentiation we compute \(z\), such that
\[
\min_{u \in L^2(\Gamma), y \in H^1(\Gamma)} J(u, y) \quad \text{subject to} \quad -\Delta \Gamma y = u - r, \quad -1 \leq u \leq 1, \quad \int_{\Gamma} y \, d\Gamma = \int_{\Gamma} u \, d\Gamma = 0
\]
is solved by
\[
\bar{u} = r = \max \left( -1, \min \left( 1, 5xyz \right) \right).
\]
As the presented tables clearly demonstrate, the examples show the expected convergence behaviour.

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