Optimal source placement as an optimal control problem in measure spaces

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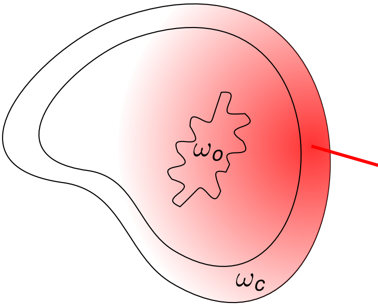
Motivation

- Optimization of light source locations in diffusive optical tomography
- Standard approach (discrete): combinatorial explosion with DOFs, requires initial set of feasible locations
- Here: Consider fictitious distributed "control field", apply sparse control techniques [Stadler '09] $\rightsquigarrow$ localization of sources
- Goal: Homogeneous illumination (application in photochemotherapy)



Sparse control problem

$$\begin{cases} \min_{u \in \mathcal{M}(\omega_c)} \frac{1}{2} \|y - z\|^2_{L^2(\omega_o)} + \alpha \|u\|_{\mathcal{M}} \\ \text{subject to } Ay = u \end{cases}$$

- $z \in L^\infty(\omega_o)$ given target
- ω_o, ω_c subdomains of $\Omega \subset \mathbb{R}^n$, $n = 2, 3$
- A linear elliptic operator
- $\mathcal{M}(\omega_c)$ space of bounded Borel measures on ω_c

Sparse control problem

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- $\|u\|_{\mathcal{M}} = \sup_{\|\varphi\|_{C_0}\leq 1} \int \varphi \, du \quad (= \|u\|_{L^1} \text{ for } u \in L^1)$
- L^1-type norms promote sparsity $\rightsquigarrow$ sparse controls
- Measure space required for well-posedness
  Alternative: control constraints
  [Stadler '09, D./G. Wachsmuth '11, Herzog/Casas/G. Wachsmuth]
- Partial observation prohibits Fenchel predual approach
- Long-term motivation: nonlinear control-to-state mapping

Problem formulation

A linear elliptic operator with appropriate boundary conditions,

Solution operator (very weak sense)

$$S_\omega : \mathcal{M}(\omega_c) \to L^2(\omega_o), \qquad u \mapsto E_{\omega_o}^* A^{-1} E_{\omega_c} u$$

Adjoint solution operator

$$S_\omega^* : L^2(\omega_o) \to C_0(\omega_c), \qquad \varphi \mapsto E_{\omega_c}^* A^{-*} E_{\omega_o} \varphi$$

E_ω extension-by-zero to Ω, E_ω^* restriction to ω

Problem formulation

$$S_\omega : \mathcal{M}(\omega_c) \to \mathrm{L}^2(\omega_o), \qquad u \mapsto E_{\omega_o}^* A^{-1} E_{\omega_c} u$$
$$S_\omega^* : \mathrm{L}^2(\omega_o) \to \mathrm{C}_0(\omega_c), \qquad \varphi \mapsto E_{\omega_c}^* A^{-*} E_{\omega_o} \varphi$$

Reduced problem

$$(\mathcal{P}) \qquad \min_{u \in \mathcal{M}(\omega_c)} \frac{1}{2} \|S_\omega u - z\|_{\mathrm{L}^2(\omega_o)}^2 + \alpha \|u\|_{\mathcal{M}}$$

Existence of minimizer from standard arguments (weak-$\star$ topology on $\mathcal{M}$)

Optimality System

$$(\mathcal{P}) \qquad \min_{u\in\mathcal{M}(\omega_c)} \frac{1}{2}\|S_\omega u - z\|^2_{L^2(\omega_o)} + \alpha\|u\|_{\mathcal{M}}$$

Theorem

Let $u^* \in \mathcal{M}(\omega_c)$ be a solution to $(\mathcal{P})$. Then there exists a $p^* \in C_0(\omega_c)$ satisfying

$$(\text{OS}) \qquad \begin{cases} S_\omega^*(S_\omega u^* - z) = p^* \\ \langle u^*, p^* - p\rangle_{\mathcal{M},C_0} \geq 0 \end{cases}$$

for all $p \in C_0(\omega_c)$ with $\|p\|_{C_0} \leq \alpha$.

Optimality System

$\mathcal{G}^*(u) := \alpha \|u\|_{\mathcal{M}}$ is Fenchel conjugate of

$$\mathcal{G} : C_0(\omega_c) \to \overline{\mathbb{R}}, \quad p \mapsto I_{\{\|p\|_{C_0} \leq \alpha\}} := \begin{cases} 0 & \text{if } \|p\|_{C_0} \leq \alpha \\ \infty & \text{else} \end{cases}$$

$\mathcal{G}^*, \mathcal{G}$ convex:

$$-S_\omega^*(S_\omega u^* - z) =: -p \in \partial\mathcal{G}^*(u) \quad \Leftrightarrow \quad u \in \partial\mathcal{G}(-p)$$

$\partial\mathcal{G}(p)$ normal cone to $I_{\{\|p\|_{C_0} \leq \alpha\}}$ at p

Regularization

Numerical solution challenging due measure space structure
$\rightsquigarrow$ consider Moreau–Yoshida regularization for $c > 0$:

Find $u_c \in L^2(\omega_c)$, $p_c \in \mathcal{W} := W_0^{2,q}(\omega_c)$, $q \in (n/2, n)$, with

$$(\mathrm{OS}_c) \qquad \begin{cases} p_c = S_\omega^*(S_\omega u_c - z) \\ -u_c = c\max(0, p_c - \alpha) + c\min(0, p_c + \alpha) \end{cases}$$

Existence: (OS_c) optimality conditions for minimizer of

$$\min_{u \in L^2(\omega_c)} \frac{1}{2}\|S_\omega u - z\|_{L^2(\omega_o)}^2 + \alpha\|u\|_{\mathcal{M}} + \frac{1}{2c}\|u\|_{L^2}^2$$

Convergence

Theorem

Let $(u_c, p_c) \in L^2(\omega_c) \times \mathcal{W}$ *be a solution of* (OS_c) *for given* $c > 0$, *and* $(u^*, p^*) \in \mathcal{M}(\omega_c) \times C_0(\omega_c)$ *a solution of* (OS). *Then we have as* $c \to \infty$*:*

$$\begin{aligned} u_c &\overset{\star}{\rightharpoonup} u^* \quad \text{in } \mathcal{M} \\ p_c &\to p^* \quad \text{in } C_0 \end{aligned}$$

$\rightsquigarrow$ Continuation strategy for $c \to \infty$

Semi-smooth Newton method

Consider (OS_c) as $F(u_c) = 0$ for $F : \mathrm{L}^2(\omega_c) \to \mathrm{L}^2(\omega_c)$,

$$F(u) = u + c\max(0, S_\omega^*(S_\omega u - z) - \alpha) \\ + c\min(0, S_\omega^*(S_\omega u - z) + \alpha)$$

$S_\omega^* : \mathrm{L}^2(\omega_o) \to \mathrm{C}_0(\omega_c) \rightsquigarrow F$ semi-smooth, chain rule:

Newton derivative

$$D_N F(u)\delta u = \delta u + c\chi_{\{|S_\omega^*(S_\omega u - z)| > \alpha\}}(S_\omega^* S_\omega \delta u)$$

($\chi_{\{|p|>\alpha\}}(x) = 1$ if $|p(x)| > \alpha$, else 0)

Semi-smooth Newton method

Semi-smooth Newton step

$$D_N F(u^k)\delta u = -F(u^k), \qquad u^{k+1} = u^k + \delta u$$

$\rightsquigarrow$ Solve by Krylov method

Theorem

For any $\alpha, c > 0$, the semi-smooth Newton method converges locally superlinearly.

("Globalization" by continuation strategy for c)

Positive controls

Control by light sources $\rightsquigarrow$ enforce positivity of controls

Set $\mathcal{G}^*(u) := I_{\{u \geq 0\}} + \|u\|_{\mathcal{M}}$:

- $\mathcal{G}(p) = I_{\{p \leq \alpha\}}$,
- $\mathcal{G}_c(p) = \frac{c}{2} \|\max(0, p - \alpha)\|_{L^2}^2$
- $\mathcal{G}_c^*(u) = I_{\{u \geq 0\}} + \alpha \|u\|_{\mathcal{M}} + \frac{1}{2c} \|u\|_{L^2}^2$

$\rightsquigarrow$ Semi-smooth Newton step for $u \in \partial \mathcal{G}_c(-p)$:

$$\delta u + c\chi_{\{S_\omega^*(S_\omega u^k - z) < -\alpha\}}(S_\omega^* S_\omega \delta u) = -u^k - c\min(0, S_\omega^*(S_\omega u - z) + \alpha)$$

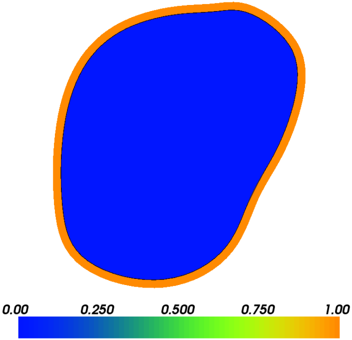
Model problem

$$\min_{y,u\geq 0} \frac{1}{2}\|y-z\|^2_{L^2(\omega_o)} + \alpha\|u\|_{\mathcal{M}(\omega_c)}$$

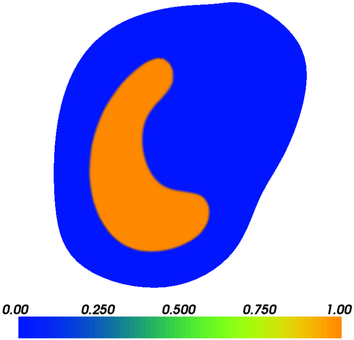
$$\text{s.t.} \begin{cases} -\nabla\cdot\left(\frac{1}{2(\mu_a+\mu_s)}\nabla y\right) + \mu_s y = E_{\omega_c} u & \text{on } \Omega, \\ \frac{1}{2(\mu_a+\mu_s)}\partial_\nu y + \rho y = 0 & \text{on } \partial\Omega \end{cases}$$

- describes diffusive light transport (e.g., in photochemotherapy)
- μ_a absorption coefficient, μ_s scattering coefficient, ρ reflection coefficient
- homogeneous illumination: $z \equiv 1$
- Finite element discretization (FEniCS) (u piecewise constant, y piecewise linear)

Example: Geometry

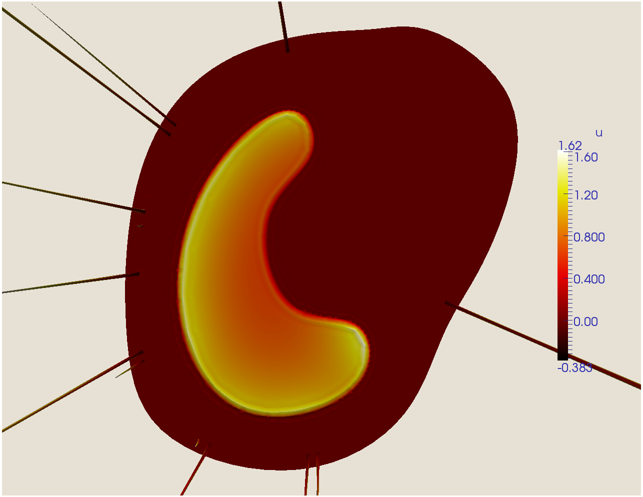


(a) control domain ω_c

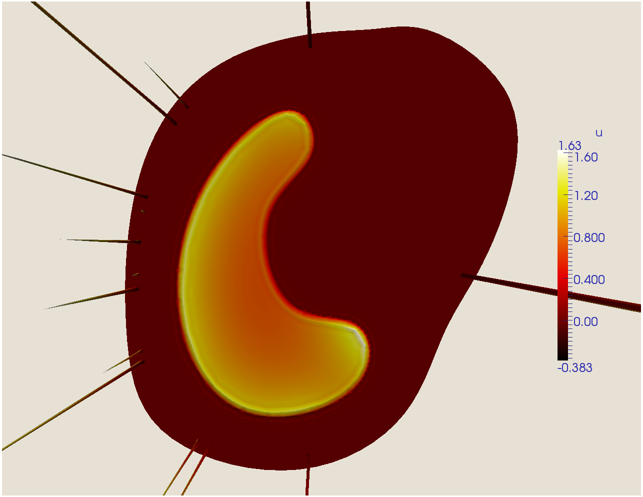


(b) observation domain ω_o

Example: $\alpha = 10^{-1}$



Example: $\alpha = 5 \cdot 10^{-2}$



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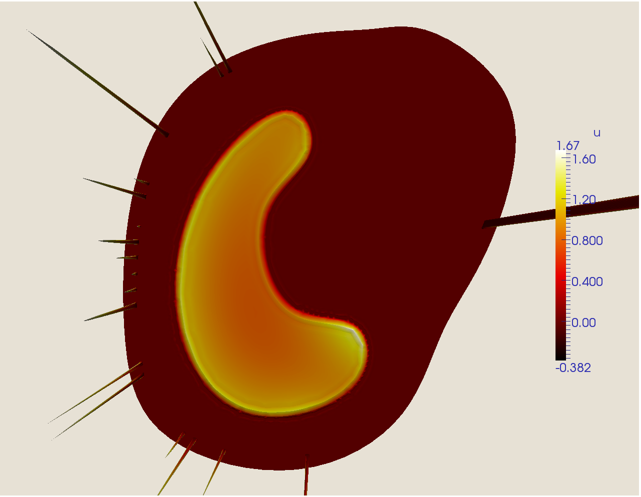
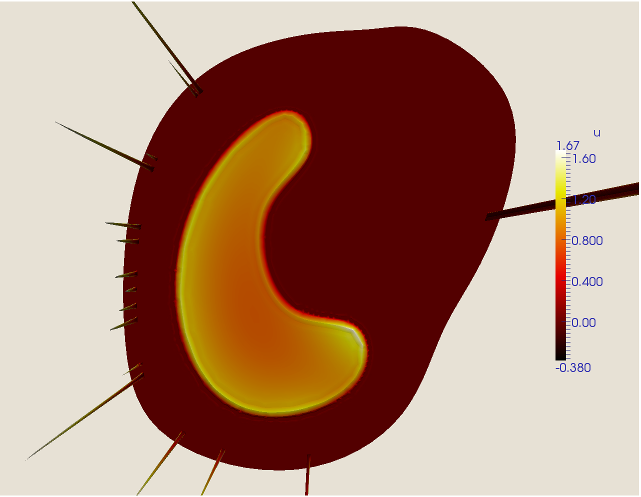


Example: $\alpha = 5 \cdot 10^{-3}$



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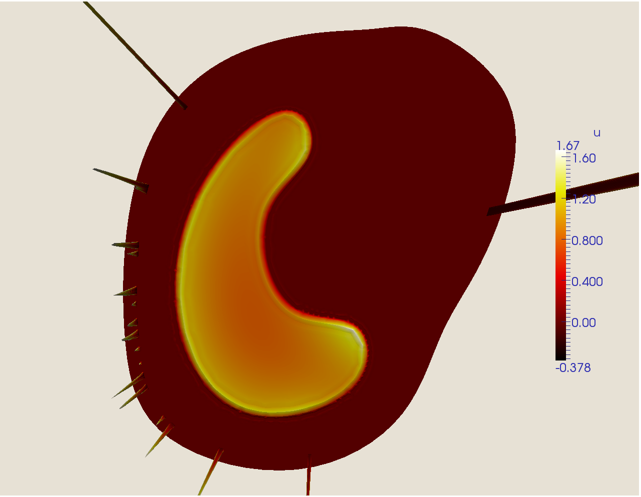
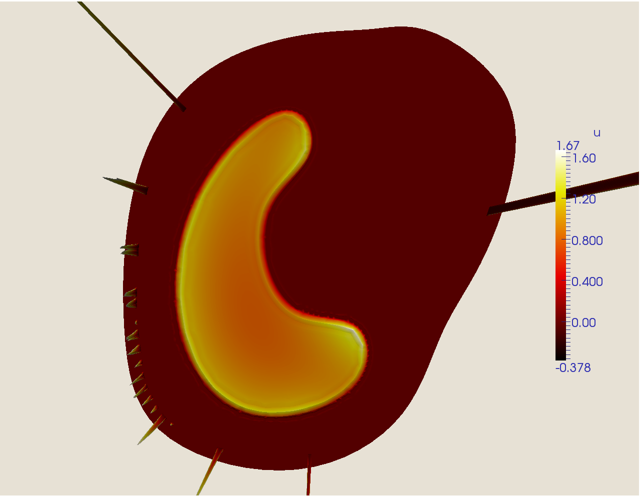
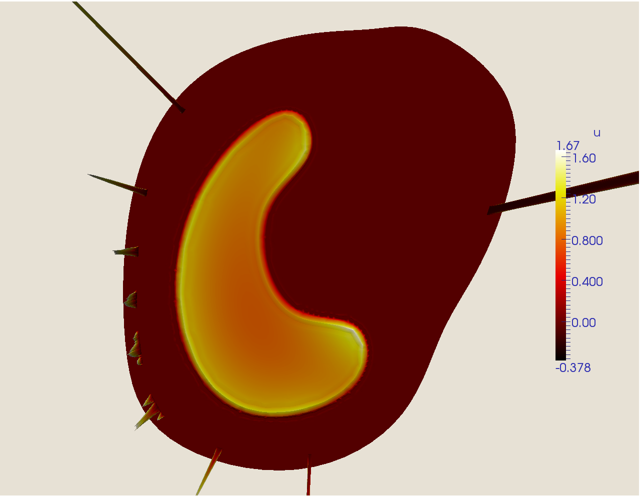


Example: $\alpha = 5 \cdot 10^{-4}$



Example: $\alpha = 10^{-4}$



Conclusion

Outlook:

- In-vivo geometry, parameters
- Nonlinear problems (approach is applicable)
- Long-term goal: Optimal experiment design in diffusive optical tomography

Cooperation partners:

Patricia Brunner, Manuel Freiberger, Hermann Scharfetter
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