A measure space approach to optimal source placement

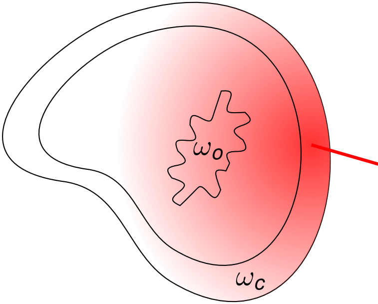
Christian Clason Karl Kunisch

Institute for Mathematics and Scientific Computing, Karl-Franzens-Universität Graz

25th IFIP TC7 Conference
Berlin, September 12, 2011

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

$$\begin{cases} \min\limits_{u \in L^1(\omega_c)} \dfrac{1}{2} \|y - z\|^2_{L^2(\omega_o)} + \alpha \|u\|_{L^1(\omega_c)} \\ \text{subject to } Ay = \chi_{\omega_c} u, \quad y|_\Gamma = 0 \end{cases}$$

- ω_o, ω_c subdomains of $\Omega \subset \mathbb{R}^n$, $n = 2, 3$; $\Gamma := \partial\Omega$
- A linear elliptic operator
- $z \in L^\infty(\omega_o)$ given target

- 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]

Sparse control problem

$$\begin{cases} \min\limits_{u \in \mathcal{M}_\Gamma(\overline{\omega}_c)} \frac{1}{2} \|y - z\|^2_{L^2(\omega_o)} + \alpha \|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)} \\ \text{subject to } Ay = \chi_{\omega_c} u, \quad y|_\Gamma = 0 \end{cases}$$

- $\mathcal{M}_\Gamma(\overline{\omega}_c)$ Radon measures with compact support on $\overline{\omega}_c \setminus \Gamma$
- topological dual of $C_\Gamma(\overline{\omega}_c) := \{v \in C(\overline{\omega}_c) : \ v|_{\partial\omega_c \cap \Gamma} = 0\}$
  ($\overline{\omega}_c \setminus \Gamma$ locally compact Hausdorff space)
- $\|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)} = \sup_{\|\varphi\|_{C_\Gamma(\overline{\omega}_c)} \leq 1} \int \varphi \, du$
  $(= \|u\|_{L^1(\omega_o)} \text{ for } u \in L^1(\omega_o))$
- Partial observation requires primal-(pre)dual approach

Problem formulation

Assumption: adjoint A^* is isomorphism from $W_0^{1,q'}(\Omega)$ to $W^{-1,q'}(\Omega) := (W_0^{1,q'}(\Omega))^*$ for $q \in (1, \frac{n}{n-1})$ and $q' = \frac{q-1}{q} \in (n, \infty)$

Then: $W_0^{1,q'}(\Omega) \hookrightarrow C_0(\overline{\Omega})$, $\mathcal{M}(\Omega) \hookrightarrow W^{-1,q}(\Omega)$ compact,

- State equation $Ay = \mu$, $y|_\Gamma = 0$, has unique solution $y \in W_0^{1,q}(\Omega)$ for every $\mu \in \mathcal{M}(\Omega)$
- Control-to-state mapping (formal definition)

$$S_\omega : \mathcal{M}_\Gamma(\overline{\omega}_c) \to L^2(\omega_o), \qquad u \mapsto (A^{-1}(\chi_{\omega_c} u))|_{\omega_o}$$

is bounded linear operator, strongly continuous:

$$u_k \rightharpoonup^* u \text{ in } \mathcal{M}_\Gamma(\overline{\omega}_c) \quad \Rightarrow \quad S_\omega(u_k) \to S_\omega(u) \text{ in } L^2(\omega_o)$$

(smooth domain and coeff's; otherwise see [Meyer/Panizzi/Schiela '10])

Problem formulation

Control-to-state mapping

$$S_\omega : \mathcal{M}_\Gamma(\overline{\omega}_c) \to L^2(\omega_o), \qquad u \mapsto (A^{-1}(\chi_{\omega_c} u))|_{\omega_o}$$

Reduced problem

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

Existence of minimizer from standard arguments (weak-$\star$ topology on $\mathcal{M}_\Gamma(\overline{\omega}_c)$)

Optimality system

Fenchel predual approach: Fenchel duality theorem yields

$$\min_{q\in L^2(\omega_o)} \frac{1}{2}\|q-z\|^2_{L^2(\omega_o)} - \frac{1}{2}\|z\|^2_{L^2(\omega_o)} + I_{\{\|v\|_{C_\Gamma(\overline{\omega}_c)}\leq\alpha\}}({}^*S_\omega q)$$
$$= \min_{u\in\mathcal{M}_\Gamma(\overline{\omega}_c)} \frac{1}{2}\|S_\omega u - z\|^2_{L^2(\omega_o)} + \alpha\|-u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)}$$

with indicator function I, “preadjoint”: $S_\omega = ({}^*S_\omega)^*$,

$${}^*S_\omega : L^2(\omega_o) \to C_\Gamma(\overline{\omega}_c), \qquad \varphi \mapsto (A^{-*}(\chi_{\omega_o})\varphi)|_{\omega_c}$$

Optimality system

Minimizers q^*, u^* satisfy extremality relations

$$\begin{cases} S_\omega u^* = q^* + z, \\ -u^* \in \partial I_{\{\|q\|_{C_\Gamma(\overline{\omega}_c)} \leq \alpha\}}({}^*S_\omega q^*). \end{cases}$$

- Introduce $p^* = {}^*S_\omega(q^*) = {}^*S_\omega(S_\omega u^* - z) \in W^{1,q'}(\omega_c)$
- Express subdifferential of indicator function (normal cone) as variational inequality

Optimality system

Theorem

Let $u^* \in \mathcal{M}_\Gamma(\overline{\omega}_c)$ *be a solution to* $(\mathcal{P})$. *Then there exists a* $p^* \in C_\Gamma(\overline{\omega}_c)$ *satisfying*

$$(\text{OS}) \qquad \begin{cases} {}^*S_\omega{}^*(S_\omega u^* - z) = p^* \\ \langle u^*, p^* - p\rangle_{\mathcal{M}_\Gamma(\overline{\omega}_c), C_\Gamma(\overline{\omega}_c)} \le 0, \quad \|p^*\|_{C_\Gamma(\overline{\omega}_c)} \le \alpha \end{cases}$$

for all $p \in C_\Gamma(\overline{\omega}_c)$ *with* $\|p\|_{C_\Gamma(\overline{\omega}_c)} \le \alpha$.

$\rightsquigarrow$ sparsity of optimal control: $\quad \operatorname{supp} u^* \subset \{x \in \overline{\omega}_c : |p^*(x)| = \alpha\}$

Non-negative Controls

Control by light sources $\rightsquigarrow$ enforce non-negativity of controls

Problem

$$\begin{cases} \min\limits_{u\in\mathcal{M}_\Gamma(\overline{\omega}_c),\, u\geq 0} \dfrac{1}{2}\|y-z\|^2_{L^2(\omega_o)} + \alpha\|u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)} \\ \text{subject to } Ay = \chi_{\omega_c}u, \quad y|_\Gamma = 0 \end{cases}$$

Non-negative Controls

Control by light sources $\rightsquigarrow$ enforce non-negativity of controls

Fenchel duality

$$\min_{q \in L^2(\omega_o)} \frac{1}{2} \|q - z\|^2_{L^2(\omega_o)} - \frac{1}{2} \|z\|^2_{L^2(\omega_o)} + I_{\{v \geq -\alpha\}}({}^* S_\omega q)$$

$$= \min_{u \in \mathcal{M}_\Gamma(\overline{\omega}_c)} \frac{1}{2} \|S_\omega u - z\|^2_{L^2(\omega_o)} + \alpha \|-u\|_{\mathcal{M}_\Gamma(\overline{\omega}_c)} + I_{\{v \leq 0\}}(-u)$$

Non-negative Controls

Control by light sources $\rightsquigarrow$ enforce non-negativity of controls

Optimality system

$$(\mathrm{OS}_+) \qquad \begin{cases} {}^*S_\omega(S_\omega u^* - z) = p^*, \\ \langle u^*, p^* - p\rangle_{\mathcal{M}_\Gamma(\overline{\omega}_c), C_\Gamma(\overline{\omega}_c)} \le 0, \qquad p^* \ge -\alpha \end{cases}$$

for all $p \in C_\Gamma(\overline{\omega}_c)$ with $p \ge -\alpha$.

Regularization

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

Find $u_c \in L^2(\omega_c)$, $p_c \in W^{1,q'}(\omega_c)$ with

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

(Here: $S_\omega : L^2(\omega_c) \to L^2(\omega_o)$, adjoint $S_\omega^*(\varphi) = {}^*S_\omega(\varphi) \in W^{1,q'}(\omega_c)$)

Alternative: Approximation by Dirac measures [Bredies/Pikkarainen '10, Casas/C/Kunisch '11]

Regularization

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

(Here: $S_\omega : \mathrm{L}^2(\omega_c) \to \mathrm{L}^2(\omega_o)$, adjoint $S_\omega^*(\varphi) = {}^*S_\omega(\varphi) \in \mathrm{W}^{1,q'}(\omega_c)$)

Existence: (OS_c) optimality conditions for minimizer of

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

Uniqueness: Strict convexity due to $\|u\|^2_{\mathrm{L}^2(\omega_c)}$

Convergence

Theorem

Let $(u_c, p_c) \in \mathrm{L}^2(\omega_c) \times \mathrm{W}^{1,q'}(\omega_c)$ *be a solution of* (OS_c) *for* $c > 0$, *then we have as* $c \to \infty$:

$$\begin{aligned} u_c &\rightharpoonup^\star u^* && \text{in } \mathcal{M}_\Gamma(\overline{\omega}_c) \\ p_c &\to p^* && \text{in } \mathrm{C}_\Gamma(\overline{\omega}_c) \end{aligned}$$

(subsequentially) to solution $(u^*, p^*) \in \mathcal{M}_\Gamma(\overline{\omega}_c) \times \mathrm{C}_\Gamma(\overline{\omega}_c)$ *of* (OS).

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

Non-negative controls

Regularized optimality system

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

optimality conditions for minimizer of

$$\min_{u \in L^2(\omega_c), u \geq 0} \frac{1}{2}\|S_\omega u - z\|^2_{L^2(\omega_o)} + \alpha \|u\|_{L^1(\omega_c)} + \frac{1}{2c}\|u\|^2_{L^2(\omega_c)}$$

Semi-smooth Newton method

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

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

$S_\omega^* : \mathrm{L}^2(\omega_o) \to \mathrm{W}_0^{1,q'}(\Omega) \quad \Rightarrow \quad F$ 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)

Non-negative controls

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

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

$\rightsquigarrow$ Semi-smooth Newton step

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

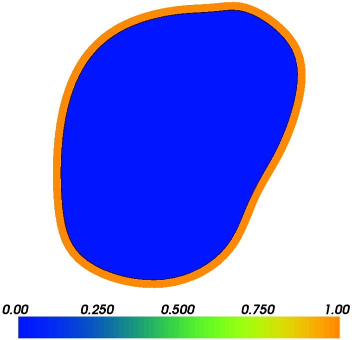
Model problem

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

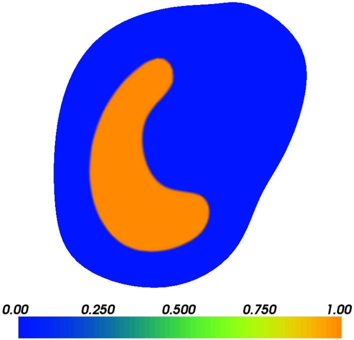
$$\text{s.t.} \begin{cases} -\nabla \cdot \left(\frac{1}{2(\mu_a+\mu_s)} \nabla y \right) + \mu_s y = \chi_{\omega_c} u & \text{on } \Omega, \\ \frac{1}{2(\mu_a+\mu_s)} \partial_\nu y + \rho y = 0 & \text{on } \partial\Omega \end{cases}$$

- 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

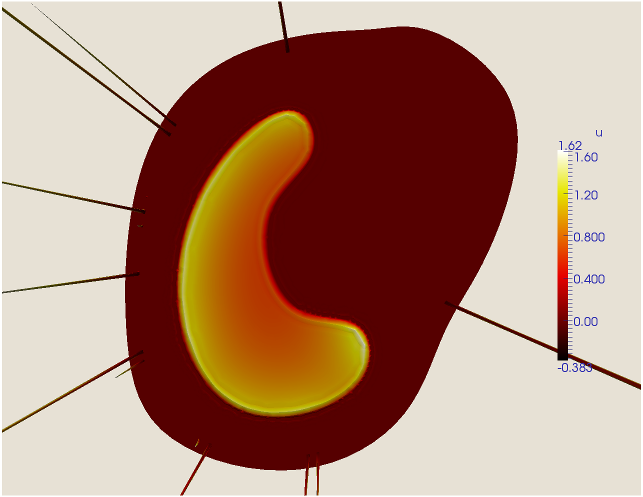


(a) control domain ω_c

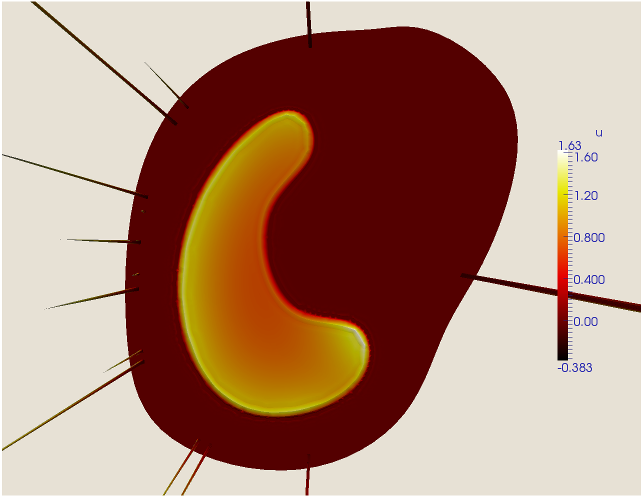


(b) observation domain ω_o

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



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



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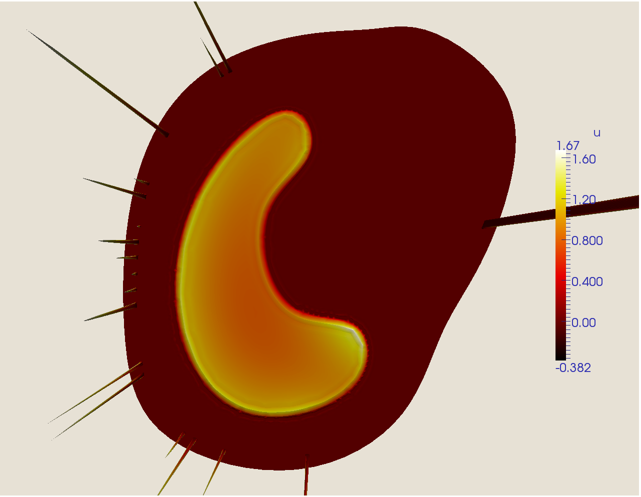
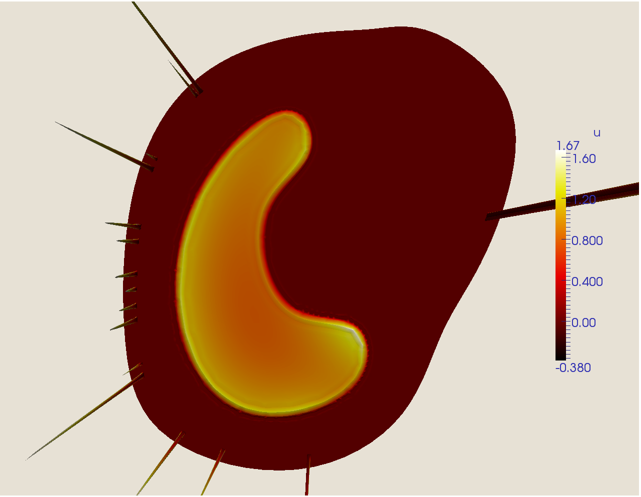


Example: $\alpha = 5 \cdot 10^{-3}$



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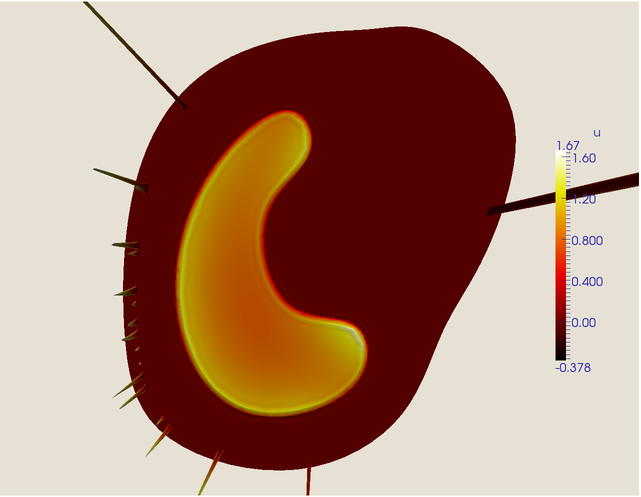
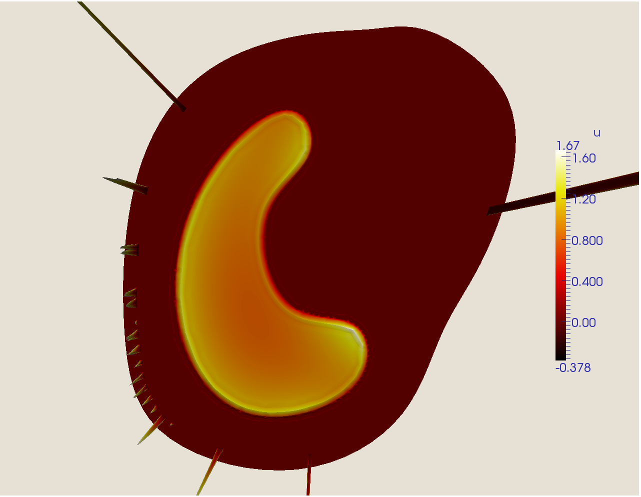
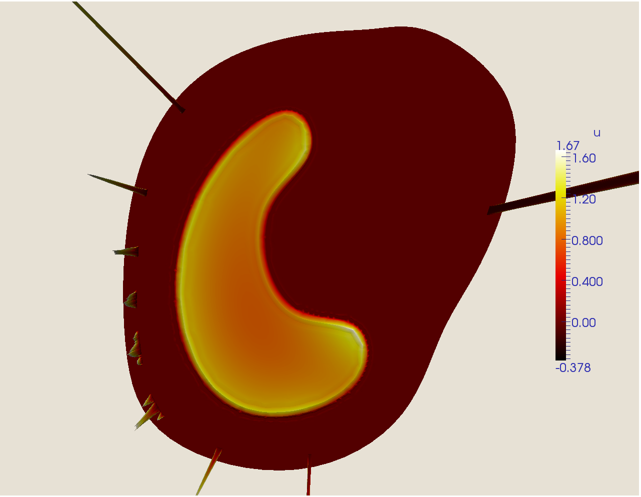


Example: $\alpha = 5 \cdot 10^{-4}$



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



Application to source placement

Measure space approach assumes

- Point sources
- Linear control costs

Not necessarily true in applications

$\rightsquigarrow$ decouple optimization of location and magnitude ("debiasing")

Application to source placement

Debiasing comparison:

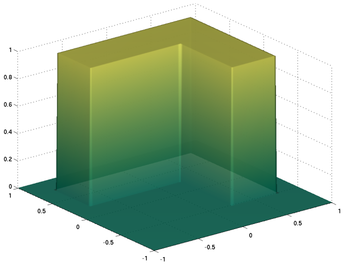
1. Solve measure space problem for large α (strong localization)
2. Select dominant "peaks", surrounding patches ω_i
3. Solve

$$\begin{cases} \min_{u\in\mathbb{R}^m} \frac{1}{2}\|y-z\|^2_{L^2(\Omega)} + \frac{\beta}{2}|u|_2^2, \\ -\Delta y = \sum_{i=1}^m \chi_{\omega_i} u_i, \quad y|_\Gamma = 0 \end{cases}$$

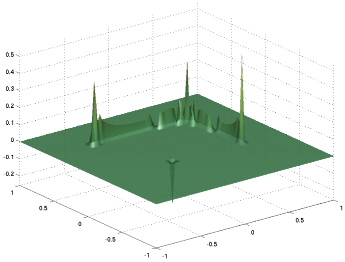
   β chosen such that $|u^*|_2 \approx M$ (given)

4. Repeat for heuristic patches (same area), same M
5. Compare tracking error $\|y^* - z\|_{L^2(\Omega)}$

Source placement: Geometry

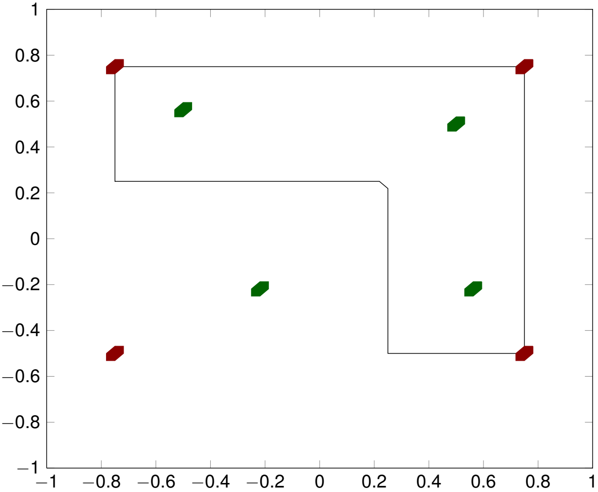


(a) target z



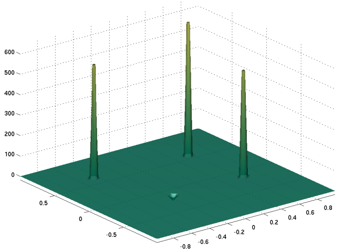
(b) sparse control

Source placement: Control patches

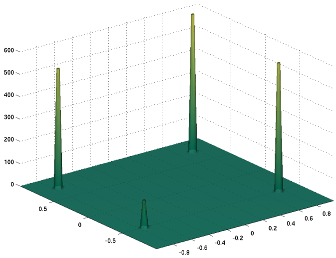


green: measure-based, red: heuristic

Source placement: Optimal controls



(a) measure-based
(tracking error 0.44843)



(b) heuristic
(tracking error 0.86210)

Conclusion

Outlook:

- Application to source placement optimization in photochemotherapy
- Nonlinear problems (approach is extendable)
- Long-term goal: Optimal experiment design in diffusive optical tomography

Cooperation partners:
Patricia Brunner, Manuel Freiberger, Hermann Scharfetter
(Institute of Medical Engineering, TU Graz)

Preprint, MATLAB code:
`http://www.uni-graz.at/~clason/publications.html`