A convex analysis approach to multi-material topology optimization

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Motivation

Topology optimization:

- optimal distribution of materials to achieve desired state
- $\rightsquigarrow$ optimal control problem for PDE with control in coefficients
- difficulty: nonlinear control-to-state mapping, nonconvex constraint (discrete set of materials)
- here: multiple (> 2) materials

Approaches:

- relaxation methods [Allaire; Bendsoe; Pironneau, Neittaanmaki]
- shape calculus [Pironneau; Sokołowski/Zolésio]
- topological calculus [Garreau; Sokołowski/Żochowski; Laurain]
- phase field [Blank]
- here: distributed coefficients [Amstutz] + penalization

Penalization

Binary penalty

$$\mathcal{G}_0(u) = \int_\Omega \frac{\alpha}{2}|u(x)|^2 + \beta \prod_{i=1}^{d} |u(x) - u_i|^0 \, dx$$

- $|t|^0 = 1$ for $t \neq 0$, $\quad |0|^0 = 0$
- "multibang" penalty [Clason/Kunisch]
- $\rightsquigarrow$ minimizer $\bar{u}(x) \in \{u_1, \dots, u_d\}$ a.e. if β large enough
- but: nonconvex, not weakly lower-semicontinuous
- $\rightsquigarrow$ consider convex envelope $\mathcal{G} := \mathcal{G}_0^{**}$

Formulation

Here: tracking-type problem

$$\min_{u\in U} \frac{1}{2}\|S(u)-z\|_Y^2 + \mathcal{G}(u)$$

- Y Hilbert space, $z \in Y$ desired state
- $U = \left\{u \in L^2(\Omega) : u(x) \in [u_1, u_d] \quad \text{for a. a. } x \in \Omega\right\}$
- S coefficient-to-state mapping, here: $u \mapsto y$,

$$\begin{cases} -\Delta y + uy = f \\ \partial_\nu y = 0 \end{cases} \quad \text{or} \quad \begin{cases} -\nabla \cdot (u\nabla y) = f \\ y = 0 \end{cases}$$

Problem statement

$$\min_{u \in U} \frac{1}{2} \|S(u) - z\|_Y^2 + \mathcal{G}(u)$$

Assumptions:

- $S : U \to Y$ is weakly continuous
- S is twice Fréchet differentiable
- $\mathcal{G} = \mathcal{G}_0^{**}$ biconjugate, i.e., conjugate of

$$\mathcal{G}_0^* : L^2(\Omega) \to \overline{\mathbb{R}}, \qquad \mathcal{G}_0^*(q) = \sup_{u \in L^2(\Omega)} \langle q, u \rangle - \mathcal{G}_0(u)$$

Existence

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$$\min_{u\in U} \frac{1}{2}\|S(u)-z\|_Y^2 + \mathcal{G}(u)$$

- $\mathcal{F}$ weakly lower-semicontinuous, bounded from below
- $\mathcal{G}$ weakly lower-semicontinuous, bounded from below, coercive since $\operatorname{dom}\mathcal{G} = U = \overline{U} = \operatorname{dom}\mathcal{G}_0$
- $\rightsquigarrow$ existence of solution $\bar u \in U$ for any $\alpha, \beta > 0$

- $\mathcal{G} \leqslant \mathcal{G}_0$, $\mathcal{G}(u) = \mathcal{G}_0(u)$ if u "multibang" ($u(x) \in \{u_1, \dots, u_d\}$ a.e.)
- $\rightsquigarrow$ $\bar u$ multibang $\Rightarrow$ $\bar u$ minimizer of $\mathcal{F} + \mathcal{G}$

Optimality conditions

- $\mathcal{F}, S$ Fréchet differentiable
- $\mathcal{G}$ convex
- $\rightsquigarrow$ existence of $\bar{p} \in L^2(\Omega)$ satisfying

primal-dual optimality system

$$\begin{cases} -\bar{p} = S'(\bar{u})^*(S(\bar{u}) - z) \\ \bar{u} \in \partial\mathcal{G}^*(\bar{p}) \end{cases}$$

- $\mathcal{G}^* = \mathcal{G}_0^* \rightsquigarrow$ explicit characterization, $\mathcal{G}$ not needed

Nonconvex penalty

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Binary penalty

$$\mathcal{G}_0(u) = \int_\Omega \frac{\alpha}{2}|u(x)|^2 + \beta \prod_{i=1}^{d} |u(x) - u_i|^0 \, dx + \delta_U(u)$$

- integral function of (nonconvex) integrand $g_0 : \mathbb{R} \to \overline{\mathbb{R}}$

$$g_0(v) = \frac{\alpha}{2}|v|^2 + \beta \prod_{i=1}^{d} |v - u_i|^0 + \delta_{[u_1,u_d]}(v)$$

- $\rightsquigarrow$ compute conjugates, subdifferential pointwise

Fenchel conjugate

$$g^*(q) = \begin{cases} qu_i - \frac{\alpha}{2}u_i^2 & q \in \overline{Q}_i, \quad 1 \leqslant i \leqslant d \\ \frac{1}{2\alpha}q^2 - \beta & q \in \overline{Q}_0 \end{cases}$$

$$Q_1 := \left\{ q : q - \alpha u_1 < \sqrt{2\alpha\beta} \wedge q < \frac{\alpha}{2}(u_1 + u_2) \right\}$$

$$Q_i := \left\{ q : |q - \alpha u_i| < \sqrt{2\alpha\beta} \wedge \frac{\alpha}{2}(u_{i-1} + u_i) < q < \frac{\alpha}{2}(u_i + u_{i+1}) \right\}$$

$$Q_d := \left\{ q : q - \alpha u_d > \sqrt{2\alpha\beta} \wedge \frac{\alpha}{2}(u_d + u_{d-1}) < q \right\}$$

$$Q_0 := \left\{ q : |q - \alpha u_j| > \sqrt{2\alpha\beta} \text{ for all } j \wedge \alpha u_1 < q < \alpha u_d \right\}$$

Subdifferential

- β sufficiently large that

$$\frac{\alpha}{2}(u_{i+1} - u_i) \leqslant \sqrt{2\alpha\beta} \quad \text{for all } 1 \leqslant i < d$$

- $\rightsquigarrow Q_0 = \emptyset$
- $\rightsquigarrow v \in \partial g_0^*(q)$ iff

$$v \in \begin{cases} \{u_1\} & q < \frac{\alpha}{2}(u_1 + u_2) \\ \{u_i\} & \frac{\alpha}{2}(u_{i-1} + u_i) < q < \frac{\alpha}{2}(u_i + u_{i+1}) \qquad 1 < i < d \\ \{u_d\} & q > \frac{\alpha}{2}(u_{d-1} + u_d) \\ [u_i, u_{i+1}] & q = \frac{\alpha}{2}(u_i + u_{i+1}) \qquad 1 \leqslant i < d \end{cases}$$

Biconjugate

- $g = g_0^{**}$ biconjugate
- biconjugate is lower convex envelope

$$g_0^{**}(v) = \begin{cases} \frac{\alpha}{2}\left((u_i + u_{i+1})v - u_i u_{i+1}\right) & v \in [u_i, u_{i+1}] \quad 1 \leqslant i < d \\ \infty & v \in \mathbb{R} \setminus [u_1, u_d] \end{cases}$$

- $\rightsquigarrow g(u_i) = g_0(u_i) = \frac{\alpha}{2} u_i^2$
- $\rightsquigarrow g$ unique function with
  1. g continuous
  2. g piecewise affine on $[u_i, u_{i+1}]$
  3. $g(u_i) = \frac{\alpha}{2} u_i^2$

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g unique function with

1. g continuous
2. g piecewise affine on $[u_i, u_{i+1}]$
3. $g(u_i) = \frac{\alpha}{2} u_i^2$

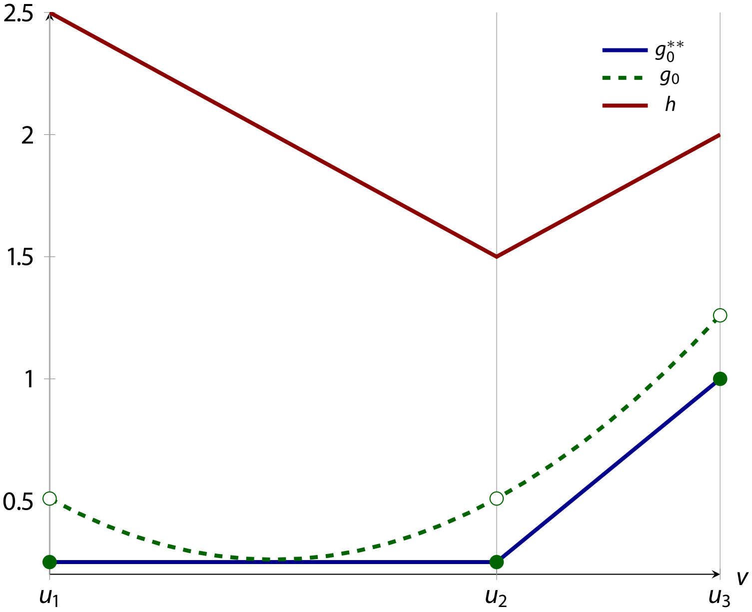
Alternatives:

- $g(u_i) = \alpha |u_i| \quad \rightsquigarrow \quad g$ shifted l_1-norm, only "kink" at $v = \min_i |u_i|$
- direct l^1 penalization

$$h(v) = \alpha \sum_{i=1}^{d} |v - u_i| + \delta_{[u_1, u_d]}(v)$$

(note: $\prod_{i=1}^{d} |v - u_i|$ polynomial of order $d \rightsquigarrow$ not convex)

Other penalizations



Other penalizations

Subdifferential of conjugate:

$$\partial h^*(q) = \begin{cases} \{u_1\} & \frac{1}{\alpha}q < 2 - d \\ \{u_i\} & 2(i-1) - d < \frac{1}{\alpha}q < 2i - d \quad 1 < i < d \\ \{u_d\} & \frac{1}{\alpha}q > d - 2 \\ [u_i, u_{i+1}] & \frac{1}{\alpha}q = 2i - d \quad 1 \leqslant i < d \end{cases}$$

$\rightsquigarrow$ undesirable properties:

- case distinction independent of u_i
- value of $\partial h^*(q)$ dependent of d
- favors $u_{d/2}$ instead of u_1

Optimality system

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$$
\begin{cases}
-\bar{p} = S'(\bar{u})^*(S(\bar{u}) - z) \\
\bar{u}(x) \in \begin{cases}
\{u_1\} & \bar{p}(x) < \frac{\alpha}{2}(u_1 + u_2) \\
\{u_i\} & \frac{\alpha}{2}(u_{i-1} + u_i) < \bar{p}(x) < \frac{\alpha}{2}(u_i + u_{i+1}) \qquad 1 < i < d \\
\{u_d\} & \bar{p}(x) > \frac{\alpha}{2}(u_{d-1} + u_d) \\
[u_i, u_{i+1}] & \bar{p}(x) = \frac{\alpha}{2}(u_i + u_{i+1}) \qquad 1 \leqslant i < d
\end{cases}
\end{cases}
$$

- set-valued $\rightsquigarrow$ not differentiable
- $\rightsquigarrow$ regularization
- but: $\mathcal{F}$ not convex $\rightsquigarrow$ regularize functional

Regularization

$$\min_{u \in L^2(\Omega)} \mathcal{F}(u) + \mathcal{G}(u) + \frac{\gamma}{2}\|u\|^2_{L^2(\Omega)}$$

- unique global minimizer $u_\gamma \in L^2(\Omega)$ for $\gamma > 0$
- $\{u_\gamma\}_{\gamma>0}$ contains sequence converging to global minimizer $\bar{u}$
- strong convergence $u_{\gamma_n} \to \bar{u}$
- optimality conditions for $\mathcal{G}_\gamma := \mathcal{G} + \frac{\gamma}{2}\|\cdot\|$

$$\begin{cases} -p_\gamma = S'(u_\gamma)^*(S(u_\gamma) - z) \\ u_\gamma \in \partial(\mathcal{G}_\gamma)^*(p_\gamma) \end{cases}$$

- $H_\gamma := \partial(\mathcal{G}_\gamma)^* = (\partial\mathcal{G}^*)_\gamma$ Moreau–Yosida regularization of $\partial\mathcal{G}^*$

Regularization

- $H_\gamma := \partial(\mathcal{G}_\gamma)^* = (\partial\mathcal{G}^*)_\gamma$ Moreau–Yosida regularization of $\partial\mathcal{G}^*$
- $\rightsquigarrow$ for β sufficiently large [Clason/Ito/Kunisch '14]

$$[H_\gamma(p)](x) = \begin{cases} u_i & p(x) \in Q_i^\gamma \quad 1 \leqslant i \leqslant d \\ \frac{1}{\gamma}\left(p(x) - \frac{\alpha}{2}(u_i + u_{i+1})\right) & p(x) \in Q_{i,i+1}^\gamma \quad 1 \leqslant i < d \end{cases}$$

$$Q_1^\gamma = \left\{q : q < \tfrac{\alpha}{2}\left(\left(1 + \tfrac{2\gamma}{\alpha}\right)u_1 + u_2\right)\right\}$$

$$Q_i^\gamma = \left\{q : \tfrac{\alpha}{2}\left(u_{i-1} + \left(1 + \tfrac{2\gamma}{\alpha}\right)u_i\right) < q < \tfrac{\alpha}{2}\left(\left(1 + \tfrac{2\gamma}{\alpha}\right)u_i + u_{i+1}\right)\right\}$$

$$Q_d^\gamma = \left\{q : \tfrac{\alpha}{2}\left(u_{d-1} + \left(1 + \tfrac{2\gamma}{\alpha}\right)u_d\right) < q\right\}$$

$$Q_{i,i+1}^\gamma = \left\{q : \tfrac{\alpha}{2}\left(\left(1 + \tfrac{2\gamma}{\alpha}\right)u_i + u_{i+1}\right) \leqslant q \leqslant \tfrac{\alpha}{2}\left(u_i + \left(1 + \tfrac{2\gamma}{\alpha}\right)u_{i+1}\right)\right\}$$

Semismooth Newton method

Pointwise computation:

- $[H_\gamma(p)](x) = h_\gamma(p(x))$
- h_γ Lipschitz continuous, piecewise C^1 $\rightsquigarrow$ semismooth
- $\rightsquigarrow$ H_γ semismooth from $L^r(\Omega)$ to $L^2(\Omega)$ iff $r > 2$
- Newton derivative

$$[D_N H_\gamma(p)h](x) = \begin{cases} \frac{1}{\gamma} h(x) & \text{if } p(x) \in Q^\gamma_{i,i+1} \quad 1 \leqslant i < d \\ 0 & \text{else} \end{cases}$$

- norm gap, bounded invertibility? $\rightsquigarrow$ structure of S

Potential problem

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Here: $y = S(u)$ satisfies

$$\begin{cases} -\Delta y + uy = f & \text{in } \Omega \\ \partial_\nu y = 0 & \text{on } \partial\Omega \end{cases}$$

- assumption: $\Omega \subset \mathbb{R}^N$, $N \leqslant 3$, sufficiently regular that

$$\|y\|_{H^2(\Omega)} \leqslant C_M \|f\|_{L^2(\Omega)}$$

- $p = S'(u)^* h = yw, \quad w$ satisfies adjoint equation

$$\begin{cases} -\Delta w + uw = -h & \text{in } \Omega \\ \partial_\nu w = 0 & \text{on } \partial\Omega \end{cases}$$

- $\rightsquigarrow y, w$ bounded in $L^\infty(\Omega)$ uniformly in $u \in U_M$

Reduced optimality system

Insert $p_\gamma = y_\gamma w_\gamma$, eliminate u_γ:

$$\begin{cases} -\Delta w_\gamma + H_\gamma(-y_\gamma w_\gamma) w_\gamma + y_\gamma = z \\ -\Delta y_\gamma + H_\gamma(-y_\gamma w_\gamma) y_\gamma = f \end{cases}$$

- $\rightsquigarrow$ equation from $H^2(\Omega) \times H^2(\Omega)$ to $L^2(\Omega) \times L^2(\Omega)$
- $\rightsquigarrow$ semismooth, partial Newton derivatives

$$D_{N,y} H_\gamma(-yw)\delta y = -\tfrac{1}{\gamma}\chi(-yw)\, w\, \delta y$$
$$D_{N,w} H_\gamma(-yw)\delta w = -\tfrac{1}{\gamma}\chi(-yw)\, y\, \delta w$$

$\chi(v)$ indicator function of $\mathcal{S}_\gamma(v) := \bigcup_{i=1}^{d-1} \left\{x \in \Omega : v(x) \in Q^\gamma_{i,i+1}\right\}$

Newton system

$$\begin{pmatrix} 1-\frac{1}{\gamma}\chi^k(w^k)^2 & -\Delta + H_\gamma(-y^kw^k) - \frac{1}{\gamma}\chi^k y^k w^k \\ -\Delta + H_\gamma(-y^kw^k) - \frac{1}{\gamma}\chi^k y^k w^k & -\frac{1}{\gamma}\chi^k(y^k)^2 \end{pmatrix} \begin{pmatrix} \delta y \\ \delta w \end{pmatrix} = -\begin{pmatrix} -\Delta w^k + H_\gamma(-y^kw^k)w^k + y^k - z \\ -\Delta y^k + H_\gamma(-y^kw^k)y^k - f \end{pmatrix}$$

- uniformly invertible if either
  1. small w_γ (small residual)
  2. $|\partial S_\gamma(-y_\gamma w_\gamma)| = 0$ (pure multibang), Schur complement invertible (1 not eigenvalue)
- continuity of H_γ, perturbation argument $\rightsquigarrow$ superlinear convergence of semismooth Newton method

Numerical example

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- finite differences, $\Omega = [-1, 1]^2$,

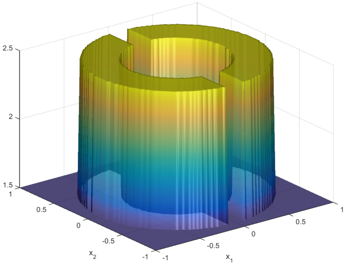
$$f(x_1, x_2) = \sin(\pi x_1)\cos(\pi x_2)$$

- fix reference coefficient

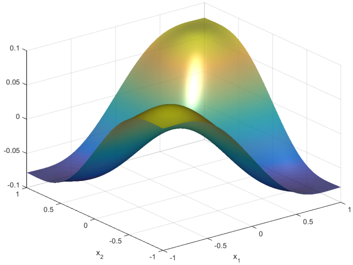
$$u_r(x_1, x_2) = \begin{cases} 2.5 & \text{if } 1/4 < |x|^2 < \frac{3}{4} \text{ and } x_1 > \frac{1}{10}, \\ 2.5 & \text{if } 1/4 < |x|^2 < \frac{3}{4} \text{ and } x_1 < -\frac{1}{10}, \\ 1.5 & \text{else}, \end{cases}$$

- target $z := y_r$ corresponding state
- extend feasible parameter set to $\{1, 1.5, 2, 2.5\}$
- compute control ($\alpha = 10^{-6}$, continuation for $\gamma \to 0$)

Numerical example

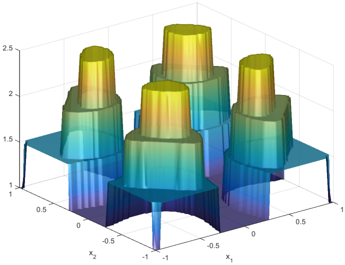


(a) reference u_r

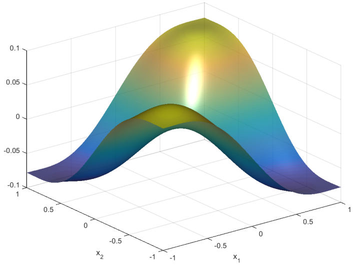


(b) target $z = y_r$

Numerical example



(c) control u_γ



(d) state y_γ

Diffusion problem

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Here: $S : u \mapsto y$ solving

$$-\nabla \cdot (u \nabla y) = f$$

- difficulty: $\bar{u} \in L^\infty(\Omega) \quad \rightsquigarrow \quad S$ not weakly-$*$ closed
  1. lack of existence of minimizer ($\bar{y} \neq S(\bar{u})$, cf. homogenization)
  2. lack of convergence $\gamma \to 0$
  3. lack of Newton differentiability of H_γ (no norm gap)
- remedies: higher regularity of y or u by
  - local smoothing: consider $\quad -\nabla \cdot \left(\int_{B_\varepsilon(x)} u(s)\, ds \nabla y \right)$
  - adding BV regularization $\|Du\|_{\mathcal{M}}$

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Local smoothing: $y = S(u)$ satisfies

$$\begin{cases} -\nabla \cdot (Gu\, \nabla y) = f & \text{in } \Omega \\ y = 0 & \text{on } \partial\Omega \end{cases}$$

- $G(u) = \frac{1}{\pi\varepsilon^2} \int_{B_\varepsilon(x)} u(s)\, ds$
- $G(L^s(\Omega)) \subset W^{1,s}(\Omega)$ for $s > N$
- $\Omega \subset \mathbb{R}^N$, $N \leqslant 3$, sufficiently regular that

$$\|y\|_{W^{2,s}(\Omega)} \leqslant C_M \|f\|_{L^s(\Omega)}$$

- $\rightsquigarrow$ adjoint state $w \in W^{2,s}(\Omega)$ with $\nabla y \cdot \nabla w \in W^{1,s}(\Omega)$

Reduced optimality system

$$\begin{cases} -\nabla \cdot \left(\left(GH_\gamma(-G^*(\nabla y_\gamma \cdot \nabla w_\gamma)) \right) \nabla w_\gamma \right) + y_\gamma = z \\ -\nabla \cdot \left(\left(GH_\gamma(-G^*(\nabla y_\gamma \cdot \nabla w_\gamma)) \right) \nabla y_\gamma \right) = f \end{cases}$$

- equation from $(W^{2,s}(\Omega) \cap H_0^1(\Omega))^2$ to $L^s(\Omega)^2$
- $\rightsquigarrow$ semismooth, Newton derivatives
- Newton system uniformly invertible if both
  1. small data (w_γ small)
  2. $|\partial S_\gamma(-G^*(\nabla y_\gamma \cdot \nabla w_\gamma)| = 0$ (pure multibang)
- $\rightsquigarrow$ superlinear convergence of semismooth Newton method

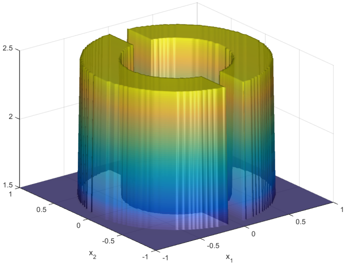
Numerical example

- finite differences, $\Omega = [-1,1]^2$, $f(x_1,x_2) = 10$
- G as local averaging over 5-point stencil
- fix reference coefficient

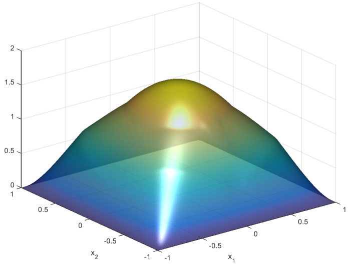
$$u_r(x_1,x_2) = \begin{cases} 2.5 & \text{if } 1/4 < |x|^2 < \frac{3}{4} \text{ and } x_1 > \frac{1}{10}, \\ 2.5 & \text{if } 1/4 < |x|^2 < \frac{3}{4} \text{ and } x_1 < -\frac{1}{10}, \\ 1.5 & \text{else,} \end{cases}$$

- target $z := y_r$ corresponding state
- extended feasible parameter set to $\{1.5, 1.75, 2, 2.25, 2.5\}$
- compute control ($\alpha = 10^{-3}$, continuation for $\gamma \to 0$)

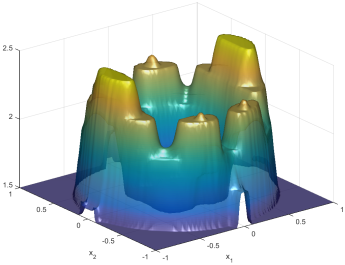
Numerical example



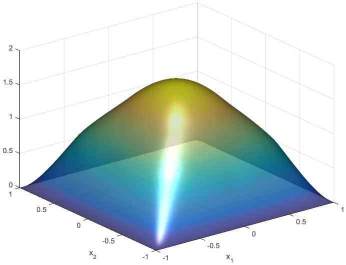
(a) reference u_r



(b) target $z = y_r$



(c) coefficient Gu_γ



(d) state y_γ

Conclusion

Convex penalization of multi-material topology optimization:

- well-posed primal-dual optimality system
- penalization exact if multi-bang solution
- linear complexity in number of parameter values
- $\rightsquigarrow$ efficient numerical solution (superlinear convergence)

Outlook:

- BV regularization (done in linear case)
- different weighting of parameter values
- other hybrid discrete–continuous problems

Preprint, MATLAB codes:

`http://www.uni-due.de/mathematik/agclason/clason_pub.php`