Optimality criteria method for multiple state optimal design problems

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Compliance maximization

State equation ($\Omega \subseteq \mathbf{R}^d$ open and bounded)

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}\nabla u) = 1 = f \\ u \in \mathrm{H}^1_0(\Omega) \end{cases}$$

$\mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}$, $\chi \in \mathrm{L}^\infty(\Omega; \{0,1\})$, $0 < \alpha < \beta$
Cost functional:

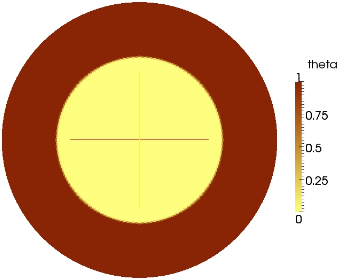
$$J(\chi) = \int_\Omega u(\mathbf{x})d\mathbf{x} \longrightarrow \max$$

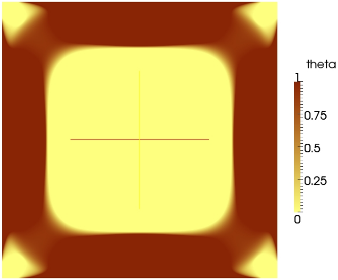
$$\int_\Omega f(\mathbf{x})u(\mathbf{x})\,d\mathbf{x} \longrightarrow \max$$

Interpretations:

- Maximize the amount of heat kept inside body
- Maximize the torsional rigidity of a rod made of two materials
- Maximize the flow rate of two viscous immiscible fluids through pipe

Ω ... circle / square





In general, there might exist no classical optimal design. The relaxation is needed, introducing composite materials

$$\chi \in \mathrm{L}^\infty(\Omega; \{0,1\}) \quad \cdots \quad \begin{array}{l} \theta \in \mathrm{L}^\infty(\Omega; [0,1]) \\ \mathbf{A} \in \mathcal{K}(\theta) \quad \text{ae on } \Omega \end{array}$$

Effective conductivities – set $\mathcal{K}(\theta)$

$\mathcal{K}(\theta)$ is given in terms of eigenvalues (Murat & Tartar; Lurie & Cherkaev):

$$\lambda_\theta^- \leq \lambda_j \leq \lambda_\theta^+ \quad j = 1, \dots, d$$

$$\sum_{j=1}^{d} \frac{1}{\lambda_j - \alpha} \leq \frac{1}{\lambda_\theta^- - \alpha} + \frac{d-1}{\lambda_\theta^+ - \alpha}$$

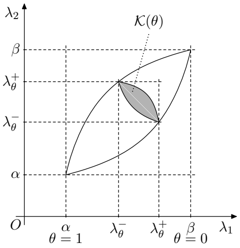
$$\sum_{j=1}^{d} \frac{1}{\beta - \lambda_j} \leq \frac{1}{\beta - \lambda_\theta^-} + \frac{d-1}{\beta - \lambda_\theta^+},$$

where

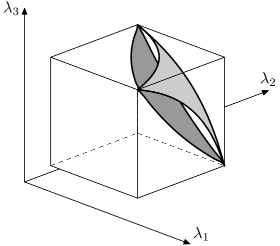
$$\lambda_\theta^+ = \theta\alpha + (1-\theta)\beta$$

$$\frac{1}{\lambda_\theta^-} = \frac{\theta}{\alpha} + \frac{1-\theta}{\beta}$$

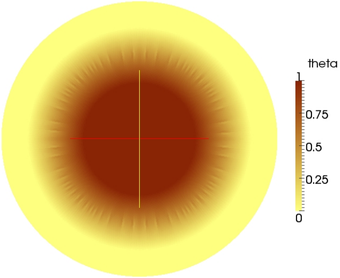
2D:

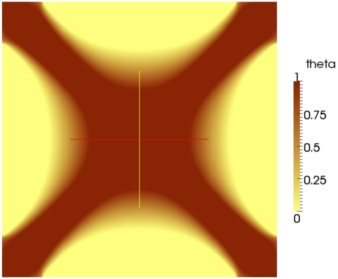


3D:



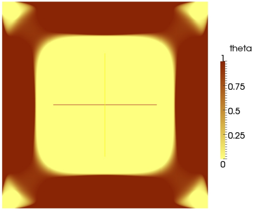
Compliance minimization

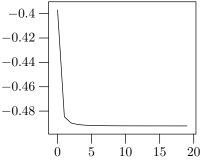




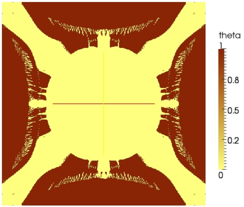
Solutions for minimization/maximization are obtained by the optimality criteria method (OCM) – actually, two variants of the method: each is good for one, but inadequate for the other problem.

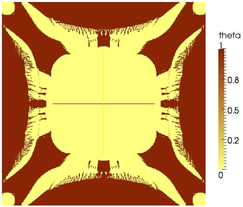
Wrong choice of the variant

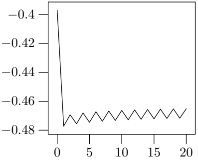




Second variant:







Important questions

To set up the method (its variants) for more complicated problems

- General cost functionals
- Multiple state optimal design problems

Example (Inverse problem)

For given functions $v \in \mathrm{H}^1_0(\Omega)$ and $f \in \mathrm{H}^{-1}(\Omega)$ we seek for a characteristic function χ such that for $\mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}$ operator $-\mathrm{div}\,(\mathbf{A}\nabla\cdot)$ (from $\mathrm{H}^1_0(\Omega)$ to $\mathrm{H}^{-1}(\Omega)$) maps v to f.
We need *a number* of such pairs (v_i, f_i) and seek for a minimizer of

$$J(\chi) = \sum_{i=1}^{m} \int_\Omega (u_i - v_i)^2\, d\mathbf{x} \longrightarrow \min$$

where u_i solves

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}\nabla u_i) = f_i \\ u_i \in \mathrm{H}^1_0(\Omega) \end{cases}$$

$->$ multiple state optimal design problem

Multiple state optimal design problem

State equations

$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla u_i) = f_i \\ u_i \in \mathrm{H}^1_0(\Omega) \end{cases} \qquad i = 1, \dots, m$$

$\mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}\,, \quad \chi \in \mathrm{L}^\infty(\Omega; \{0,1\})$

State function $\mathrm{u} = (u_1, \dots, u_m)$

$$\begin{aligned} J(\chi) &= \int_\Omega F(\mathbf{x}, \chi(\mathbf{x}), u(\mathbf{x}))\, d\mathbf{x} \\ &= \int_\Omega \Big(\chi\, g_\alpha(\cdot, \mathrm{u}) + (1-\chi)\, g_\beta(\cdot, \mathrm{u})\Big)\, d\mathbf{x} + l \int_\Omega \chi\, d\mathbf{x} \\ &= \int_\Omega \chi\, \Big(l + g_\alpha(\cdot, \mathrm{u}) - g_\beta(\cdot, \mathrm{u})\Big) + g_\beta(\cdot, \mathrm{u})\, d\mathbf{x} \to \min \end{aligned}$$

Relaxed problem: $J(\theta, \mathbf{A}) = \int_\Omega \theta\, \Big(l + g_\alpha(\cdot, \mathrm{u}) - g_\beta(\cdot, \mathrm{u})\Big) + g_\beta(\cdot, \mathrm{u})\, d\mathbf{x} \to \min$

where

$$\begin{aligned} \theta\ &\in \mathrm{L}^\infty(\Omega; [0,1]) \\ \mathbf{A}\ &\in \mathcal{K}(\theta) \quad \text{ae on } \Omega\,. \end{aligned}$$

Adjoint equations

$(\theta^*, \mathbf{A}^*)$ optimal design; consider its variation $(\delta\boldsymbol{\theta}, \delta\mathbf{A})$
Adjoint state $\mathrm{p}^* = (p_1, \dots, p_m)$

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}\nabla p_i) = \theta \frac{\partial g_\alpha}{\partial \lambda_i}(\cdot, \mathrm{u}^*) + (1-\theta)\frac{\partial g_\beta}{\partial \lambda_i}(\cdot, \mathrm{u}^*) \\ p_i \in \mathrm{H}^1_0(\Omega)\,. \end{cases} \qquad i = 1, \dots, m$$

$$\delta J = \int_\Omega \delta\boldsymbol{\theta}\big[l + g_\alpha(\cdot, \mathrm{u}^*) - g_\beta(\cdot, \mathrm{u}^*)\big] - \int_\Omega \sum_{i=1}^m \delta\mathbf{A}\nabla u_i^* \cdot \nabla p_i^* \geq 0$$

Problem: variations $\delta\boldsymbol{\theta}$ and $\delta\mathbf{A}$ are related ... $\mathbf{A} \in \mathcal{K}(\theta)$
For the moment: $\delta\boldsymbol{\theta} = 0$
First variant of OCM ... $\delta\mathbf{A} = \mathbf{A} - \mathbf{A}^*$ for some $\mathbf{A} \in \mathcal{K}(\theta^*)$:

$$\int_\Omega \sum_{i=1}^m \mathbf{A}\nabla u_i^* \cdot \nabla p_i^* \leq \int_\Omega \sum_{i=1}^m \mathbf{A}^*\nabla u_i^* \cdot \nabla p_i^*\,,\ \mathbf{A} \in \mathcal{K}(\theta^*)$$

Necessary condition of optimality

Almost everywhere on Ω the problem

$$\begin{cases} \sum_{i=1}^{m} \mathbf{A}\nabla u_i^* \cdot \nabla p_i^* \longrightarrow \max \\ \mathbf{A} \in \mathcal{K}(\theta^*) \end{cases}$$

has $\mathbf{A}^*$ as a solution.

$$\sum_{i=1}^{m} \mathbf{A}\nabla u_i^* \cdot \nabla p_i^* = \mathbf{A} \cdot \mathbf{M}^* , \quad \mathbf{M}^* = \mathrm{Sym} \sum_{i=1}^{m} \nabla u_i^* \otimes \nabla p_i^*$$

$$f(\theta, \mathbf{M}) := \max_{\mathbf{A} \in \mathcal{K}(\theta)} \mathbf{A} \cdot \mathbf{M} , \quad \theta \in [0,1] , \ \mathbf{M} \in Sym(d)$$

General $\delta\boldsymbol{\theta}$ ... a smooth path $\varepsilon \mapsto \theta_\varepsilon$ in $\mathrm{L}^\infty(\Omega; [0,1])$, $\theta_0 = \theta^*$

$\mathbf{A}_\varepsilon(\mathbf{x})$ maximizer for $f(\theta_\varepsilon(\mathbf{x}), \mathbf{M}^*(\mathbf{x}))$

Necessary condition of optimality

Theorem (Allaire, 2002)

For

$$Q(\mathbf{x}) := l + g_\alpha(\mathbf{x}, u^*(\mathbf{x})) - g_\beta(\mathbf{x}, u^*(\mathbf{x})) - \frac{\partial f}{\partial \theta}(\theta^*(\mathbf{x}), \mathbf{M}^*(\mathbf{x}))\,,$$

the optimal density θ^* satisfies

$$\begin{aligned} Q(\mathbf{x}) > 0 &\implies \theta^*(\mathbf{x}) = 0\,, \\ Q(\mathbf{x}) < 0 &\implies \theta^*(\mathbf{x}) = 1\,, \\ Q(\mathbf{x}) = 0 &\implies \theta^*(\mathbf{x}) \in [0,1]\,. \end{aligned}$$

Almost everywhere on Ω, $\mathbf{A}^*$ is the maximizer in the definition of $f(\theta^*, \mathbf{M}^*)$.

In the following, we write $\mathcal{K}(\alpha, \beta; \theta)$ instead of $\mathcal{K}(\theta)$ and f_α^β instead of f:

$$f_\alpha^\beta(\theta, \mathbf{M}) = \max_{\mathbf{A} \in \mathcal{K}(\alpha,\beta;\theta)} \mathbf{A} \cdot \mathbf{M}\,.$$

Optimality criteria method – first variant

New design $(\theta^{k+1}, \mathbf{A}^{k+1})$ is defined by optimality condition.

1. Calculate $\mathrm{u}^k = (u_1, \ldots, u_m)$, the solution of

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}^k \nabla u_i) = f_i \\ u_i \in \mathrm{H}_0^1(\Omega)\,. \end{cases} \qquad i = 1, \ldots, m$$

2. Calculate p^k, the solution of

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}^k \nabla p_i) = \theta^k \frac{\partial g_\alpha}{\partial u_i}(\cdot, \mathrm{u}^k) + (1-\theta^k)\frac{\partial g_\beta}{\partial u_i}(\cdot, \mathrm{u}^k) \\ p_i \in \mathrm{H}_0^1(\Omega) \end{cases} \qquad i = 1, \ldots, m$$

   and $\mathbf{M}^k = \mathrm{Sym} \sum_{i=1}^m \nabla u_i^k \otimes \nabla p_i^k$

3. For $\mathbf{x} \in \Omega$, let $\theta^{k+1}(\mathbf{x})$ be the zero of function

$$\theta \mapsto l + g_\alpha(\mathbf{x}, \mathrm{u}^k(\mathbf{x})) - g_\beta(\mathbf{x}, \mathrm{u}^k(\mathbf{x})) - \frac{\partial}{\partial\theta} f_\alpha^\beta(\theta, \mathbf{M}^k(\mathbf{x}))\,,$$

   (if zero doesn't exist, take 0 (or 1) in case the function is positive (or < 0)) and $\mathbf{A}^{k+1}(\mathbf{x})$ be the maximizer in the definition of $f(\theta^{k+1}(\mathbf{x}), \mathbf{M}^k(\mathbf{x}))$.

Design update

Theorem

For given $\theta \in [0,1]$ and matrix $\mathbf{M}$ with eigenvalues $\mu_1 \le \mu_2$ we have

A. *If $\mu_2 < 0$ and $\theta > \theta^A := \left(\frac{\sqrt{-\mu_1}}{\sqrt{-\mu_2}} - 1\right)\frac{\alpha}{\beta-\alpha}$*

$$\frac{\partial}{\partial\theta} f_\alpha^\beta(\theta,\mathbf{M}) = \alpha\,\left(\beta^2-\alpha^2\right)\left(\frac{\sqrt{-\mu_1}+\sqrt{-\mu_2}}{\theta(\beta-\alpha)+2\alpha}\right)^2,$$

B. *If $\mu_1 > 0$ and $\theta < \theta^B = \left(\frac{\sqrt{\mu_1}}{\sqrt{\mu_2}} - \frac{\alpha}{\beta}\right)\frac{\beta}{\beta-\alpha}$*

$$\frac{\partial}{\partial\theta} f_\alpha^\beta(\theta,\mathbf{M}) = \beta\,\left(\beta^2-\alpha^2\right)\left(\frac{\sqrt{\mu_1}+\sqrt{\mu_2}}{\theta(\beta-\alpha)+\alpha+\beta}\right)^2,$$

C. *Else*

$$\frac{\partial}{\partial\theta} f_\alpha^\beta(\theta,\mathbf{M}) = -\frac{\alpha\,\beta\,(\beta-\alpha)\,\mu_1}{\left(\theta\,(\beta-\alpha)\,+\alpha\right)^2} - \mu_2\,(\beta-\alpha)\,.$$

We are able to introduce design update explicitly

$$\theta^{k+1} = \Psi_\theta(\alpha,\beta,l,\mathbf{M}^k)\,,\ \mathbf{A}^{k+1} = \Psi_{\mathbf{A}}(\alpha,\beta,l,\mathbf{M}^k)\,.$$

Inverse conductivities

$\mathbf{A} \in \mathcal{K}(\alpha, \beta; \theta) \quad \Longleftrightarrow \quad$ eigenvalues $\nu_1, \dots \nu_d$ of inverse matrix $\mathbf{A}^{-1}$ satisfy

$$
\begin{aligned}
\nu_\theta^+ \leq \quad \nu_j \quad &\leq \nu_\theta^- \,, \quad j = 1, \dots, d \,, \\
\sum_{j=1}^{d} \frac{1}{\alpha^{-1} - \nu_j} \quad &\leq \quad \frac{1}{\alpha^{-1} - \nu_\theta^-} + \frac{d-1}{\alpha^{-1} - \nu_\theta^+} \,, \qquad \nu_\theta^- = \frac{1}{\lambda_\theta^-} \,,\ \nu_\theta^+ = \frac{1}{\lambda_\theta^+} \,. \\
\sum_{j=1}^{d} \frac{1}{\nu_j - \beta^{-1}} \quad &\leq \quad \frac{1}{\nu_\theta^- - \beta^{-1}} + \frac{d-1}{\nu_\theta^+ - \beta^{-1}} \,,
\end{aligned}
$$

Lemma

For $d = 2$

$$
\mathbf{A} \in \mathcal{K}(\alpha, \beta; \theta) \quad \Longleftrightarrow \quad \mathbf{A}^{-1} \in \mathcal{K}\left(\frac{1}{\beta}, \frac{1}{\alpha}, 1 - \theta\right) .
$$

Variation in $\mathbf{A}$

$\delta\boldsymbol{\theta} = 0$: $\mathbf{A}(\varepsilon) = ((1-\varepsilon)\mathbf{A}^{*\,-1} + \varepsilon\mathbf{A}^{-1})^{-1}$ (for some $\mathbf{A} \in \mathcal{K}(\theta^*)$) leads to

$$\delta\mathbf{A} = \frac{d}{d\varepsilon}\mathbf{A}(\varepsilon)\Big|_{\varepsilon=0} = -\mathbf{A}^*(\mathbf{A}^{-1} - \mathbf{A}^{*\,-1})\mathbf{A}^*\,. \tag{1}$$

$-\sum_{i=1}^m \delta\mathbf{A}\nabla u_i^* \cdot \nabla p_i^* \geq 0$ means: $\mathbf{A}^*(\mathbf{x})$ solves

$$\begin{cases} \displaystyle\sum_{i=1}^m \mathbf{A}^{-1}\boldsymbol{\sigma}_i^* \cdot \boldsymbol{\tau}_i^* \to \min \\ \mathbf{A} \in \mathcal{K}(\theta^*) \end{cases} \qquad \boldsymbol{\sigma}_i^* = \mathbf{A}^*\nabla u_i^*\,,\ \boldsymbol{\tau}_i^* = \mathbf{A}^*\nabla p_i^*$$

We introduce the function $g_\alpha^\beta(\theta, \mathbf{N}) = \min\limits_{\mathbf{A}\in\mathcal{K}(\alpha,\beta;\theta)} \mathbf{A}^{-1}\cdot\mathbf{N}$

Lemma

Let $\theta \in [0,1]$ and $\mathbf{N} \in \mathbf{R}^{2\times 2}$ be a symmetric matrix. Then

$$\begin{aligned} g_\alpha^\beta(\theta,\mathbf{N}) &= -f_{1/\beta}^{1/\alpha}(1-\theta, -\mathbf{N})\,, \\ \frac{\partial g_\alpha^\beta}{\partial\theta}(\theta,\mathbf{N}) &= \frac{\partial}{\partial\theta} f_{1/\beta}^{1/\alpha}(1-\theta, -\mathbf{N})\,. \end{aligned}$$

Variation in θ

To take into account the variations in θ we proceed analogously:we take a smooth path $(\theta_\varepsilon, \mathbf{A}_\varepsilon)$ such that $\mathbf{A}_\varepsilon(\mathbf{x})$ is a minimizer for $g_\alpha^\beta(\theta_\varepsilon(\mathbf{x}), \mathbf{N}^*(\mathbf{x}))$, with $\mathbf{N}^* = \mathrm{Sym}\sum_{i=1}^m \boldsymbol{\sigma}_i^* \otimes \boldsymbol{\tau}_i^*$:

$$\mathbf{A}_\varepsilon(\mathbf{x})^{-1} \cdot \mathbf{N}^*(\mathbf{x}) = g_\alpha^\beta(\theta_\varepsilon(\mathbf{x}), \mathbf{N}^*(\mathbf{x}))\,, \quad \text{a.e. } \mathbf{x} \in \Omega\,.$$

If we take derivative in ε in the last equation, for $\varepsilon = 0$ we have (almost everywhere on Ω)

$$-\mathbf{A}^{*\,-1}\delta\mathbf{A}\mathbf{A}^{*\,-1} \cdot \sum_{i=1}^m \mathbf{A}^*\nabla u_i^* \otimes \mathbf{A}^*\nabla p_i^* = \frac{\partial}{\partial\theta} g_\alpha^\beta(\theta^*, \mathbf{N}^*)\,,$$

which implies

$$\delta\mathbf{A}\sum_{i=1}^m \nabla u_i^* \otimes \nabla p_i^* = -\frac{\partial}{\partial\theta} g_\alpha^\beta(\theta^*, \mathbf{N}^*)\,.$$

The necessary condition of optimality $\delta J \geq 0$, for the variation obtained in this way leads to the following result:

Necessary condition of optimality

Theorem

For $\mathbf{N}^* = \mathrm{Sym} \sum_{i=1}^m \boldsymbol{\sigma}_i^* \otimes \boldsymbol{\tau}_i^*$*, the optimal design* $(\theta^*, \mathbf{A}^*)$ *satisfies* $\mathbf{A}^*(\mathbf{x})^{-1} \cdot \mathbf{N}^*(\mathbf{x}) = -f_{1/\beta}^{1/\alpha}(1 - \theta_\varepsilon(\mathbf{x}), -\mathbf{N}^*(\mathbf{x}))$*, for almost every* $\mathbf{x} \in \Omega$*. Defining the quantity*

$$P(\mathbf{x}) = l + g_\alpha(\mathbf{x}, u^*(\mathbf{x})) - g_\beta(\mathbf{x}, u^*(\mathbf{x})) + \frac{\partial f_{1/\beta}^{1/\alpha}}{\partial \theta}(1 - \theta^*(\mathbf{x}), -\mathbf{N}^*(\mathbf{x})) \, ,$$

the optimal density θ^* *satisfies, almost everywhere on* Ω*,*

$$\begin{aligned} P(\mathbf{x}) > 0 \quad &\Longrightarrow \quad \theta^*(\mathbf{x}) = 0 \, , \\ P(\mathbf{x}) < 0 \quad &\Longrightarrow \quad \theta^*(\mathbf{x}) = 1 \, , \\ P(\mathbf{x}) = 0 \quad &\Longrightarrow \quad \theta^*(\mathbf{x}) \in [0, 1] \, . \end{aligned}$$

Optimality criteria method – Second variant

Take some initial θ^0 and $\mathbf{A}^0$. For k from 1 to N:

1. Calculate u_i^k, $i = 1, \ldots, m$, the solution of

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}^k \nabla u) = f_i \\ u \in \mathrm{H}_0^1(\Omega)\,. \end{cases}$$

2. Calculate p_i^k, the solution of

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}^k \nabla p) = 2(u_i - v_i) \\ p \in \mathrm{H}_0^1(\Omega)\,, \end{cases}$$

   and $\mathbf{N}^k = \mathrm{Sym} \sum_{i=1}^m (\mathbf{A}^k \nabla u_i^k \otimes \mathbf{A}^k \nabla p_i^k)$

3. For $\mathbf{x} \in \Omega$, let $\theta^{k+1}(\mathbf{x})$ be the zero of function

$$\theta \mapsto I + g_\alpha(\mathbf{x}, \mathrm{u}^k(\mathbf{x})) - g_\beta(\mathbf{x}, \mathrm{u}^k(\mathbf{x})) + \frac{\partial}{\partial \theta} f_{1/\beta}^{1/\alpha}(1-\theta, -\mathbf{N}^k(\mathbf{x}))\,, \qquad (2)$$

   if a zero doesn't exist, take 0 (or 1) in case the function is positive (or < 0). Furthermore, $\mathbf{A}^{k+1}(\mathbf{x}) = \mathbf{B}^{-1}$, where $\mathbf{B}$ is the maximizer in the definition of $f_{1/\beta}^{1/\alpha}(1-\theta^{k+1}(\mathbf{x}), -\mathbf{N}^k(\mathbf{x}))$.

Design update – Second variant

Using the result of the previous Lemma, the update of the design variables can be written in terms of update for the first variant:

$$\theta^{k+1}(\mathbf{x}) = 1 - \Psi_\theta \left(\frac{1}{\beta}, \frac{1}{\alpha}, -I, -N^k(\mathbf{x}) \right) ,$$

and

$$\mathbf{A}^{k+1}(\mathbf{x}) = \Psi_{\mathbf{A}} \left(\frac{1}{\beta}, \frac{1}{\alpha}, -I, -N^k(\mathbf{x}) \right)^{-1} .$$

Similar (but more tedious) calculation can be done for $d = 3$.

Example – Inverse problem

We start with a distribution of two materials, and for given right-hand sides $f_1, \ldots, f_m$, corresponding temperatures $v_1, \ldots, v_m$ are calculated.
The optimal design problem reads

$$J(\chi) = \sum_{i=1}^{m} \int_{\Omega} (u_i - v_i)^2 \, d\mathbf{x} \longrightarrow \min$$

where u_i solves

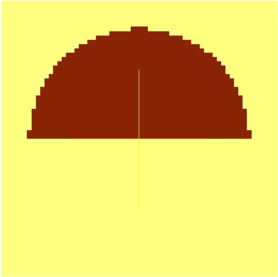
$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla u_i) = f_i \\ u_i \in \mathrm{H}_0^1(\Omega) \end{cases}$$

The aim is to recover the original distribution of materials.

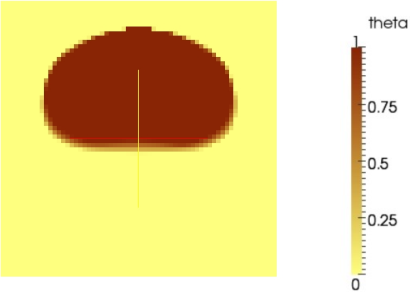
In the following examples:
$\Omega = [-1, 1]^2$, $\alpha = 1$, $\beta = 2$, $m = 8$

Numerical results 1

Exact solution



One-shoot solution

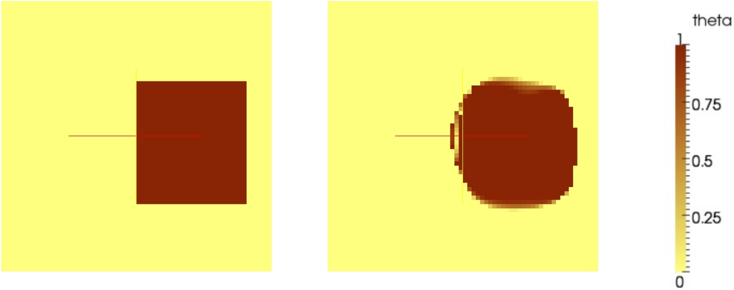


Initial iteration - homogeneous material

The value of the cost functional reduces from 0.0159 to 0.0007

Numerical results 2

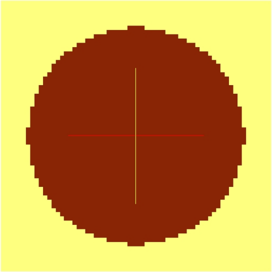
Exact solution One-shoot solution

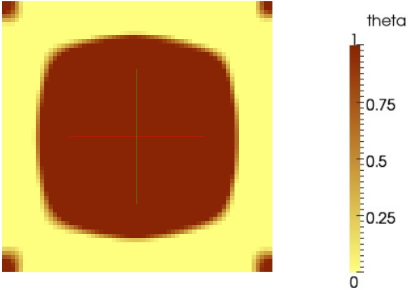


Initial iteration - homogeneous material
The value of the cost functional reduces from 0.0121 to 0.0002

Numerical results 3

Exact solution One-shoot solution





Initial iteration - homogeneous material
The value of the cost functional reduces from 0.0421 to 0.0019