Shape derivative method for optimal design in conductivity problem

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Introduction

Let $\Omega \subset \mathbb{R}^d$ be open and bounded set.
Two phases each with different isotropic conductivity: α, β $(0 < \alpha < \beta)$.
q_α is the prescribed volume of the first phase α $(0 < q_\alpha < |\Omega|)$.
$\chi \in L^\infty(\Omega)$ such that $\chi(1-\chi) = 0$.

Conductivity can be expressed as

$$\mathbf{A}(\chi) := \chi\alpha\,\mathbf{I} + (1-\chi)\beta\,\mathbf{I},$$

where

$$\int_\Omega \chi(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = q_\alpha.$$

State function $u \in \mathrm{H}_0^1(\Omega)$ is a solution of the following boundary value problem:

$$\left\{\begin{array}{cc} -\mathrm{div}(\mathbf{A}\,\nabla u) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{array}\right. \tag{1}$$

Energy functional:

$$J(\chi) := \int_\Omega f(\boldsymbol{x})u(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

Statement of the problem

Optimal design problem:

$$
(\mathrm{P}) \qquad \begin{cases} J(\chi) = \displaystyle\int_\Omega f u \, \mathrm{d}\boldsymbol{x} \to \max \\ \text{s.t.} \quad \chi \in L^\infty(\Omega, \{0,1\}), \quad \displaystyle\int_\Omega \chi \, \mathrm{d}\boldsymbol{x} = q_\alpha, \\ u \text{ solves (1) with } \mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}. \end{cases}
$$

If solution χ exists for (P) we call it *classical solution.*

Important: For general optimal design problems the classical solutions usually does not exist.

Aim of this talk:

- to present examples of classical solutions on annuli.
- solve problem numerically using shape derivative method.

Relaxed design

For characteristic functions relaxation consists of:

$$\chi \in L^\infty(\Omega, \{0,1\}) \quad \rightsquigarrow \quad \theta \in L^\infty(\Omega, [0,1]), \tag{2}$$

with

$$\int_\Omega \theta \, \mathrm{d}\boldsymbol{x} := q_\alpha .$$

Notion of H-convergence is introduced for conductivity $\mathbf{A}$.

Effective conductivities:

$$\mathcal{K}(\theta) \subset M_d(\mathbb{R}) \text{ with local fraction } \theta \in [0,1].$$

Precisely, $A \in \mathcal{K}(\theta)$ iff there exists sequence of characteristic functions

$$\begin{cases} \chi_n \xrightarrow{L^\infty \star} \theta \\ \mathbf{A}^n = \chi_n \alpha \mathbf{I} + (1-\chi_n) \beta \mathbf{I} \xrightarrow{H} A. \end{cases}$$

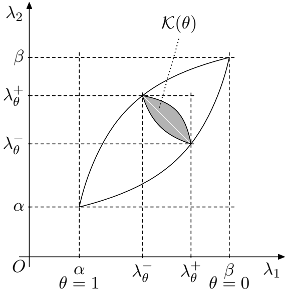
Effective conductivities - set $\mathcal{K}(\theta)$

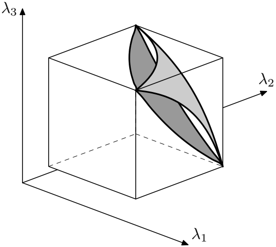
$\mathcal{K}(\theta)$ is given in terms of eigenvalues

$$
\begin{aligned}
\lambda_\theta^- \le \quad \lambda_j \quad &\le \lambda_\theta^+ \quad j = 1, \dots, d \\
\sum_{j=1}^{d} \frac{1}{\lambda_j - \alpha} \quad &\le \quad \frac{1}{\lambda_\theta^- - \alpha} + \frac{d-1}{\lambda_\theta^+ - \alpha} \\
\sum_{j=1}^{d} \frac{1}{\beta - \lambda_j} \quad &\le \quad \frac{1}{\beta - \lambda_\theta^-} + \frac{d-1}{\beta - \lambda_\theta^+},
\end{aligned}
$$

where

$$
\begin{aligned}
\lambda_\theta^+ \quad &= \quad \theta\alpha + (1-\theta)\beta \\
\frac{1}{\lambda_\theta^-} \quad &= \quad \frac{\theta}{\alpha} + \frac{1-\theta}{\beta}.
\end{aligned}
$$





Generalized (convex) problem

Relaxed design:

$$\mathcal{A} = \left\{ (\theta, \mathbf{A}) \in L^\infty(\Omega, [0,1] \times \mathrm{Sym}_d) \;\middle|\; \begin{array}{c} \int_\Omega \theta \, \mathrm{d}\boldsymbol{x} = q_\alpha, \\ \mathbf{A}(\boldsymbol{x}) \in \mathcal{K}(\theta(\boldsymbol{x})), \;\text{ a.e. } \boldsymbol{x} \end{array} \right\}$$

Relaxed problem can be written as:

$$\text{(A)} \qquad \max_{(\theta,\mathbf{A})\in\mathcal{A}} J(\theta, \mathbf{A}) = \max_{(\theta,\mathbf{A})\in\mathcal{A}} \int_\Omega f u \, \mathrm{d}\boldsymbol{x}$$

Unfortunately, $\mathcal{A}$ is not a convex set. To achieve convexity, an enlarged set is introduced:

$$\mathcal{B} = \left\{ (\theta, \mathbf{A}) \in L^\infty(\Omega, [0,1] \times \mathrm{Sym}_d) \;\middle|\; \begin{array}{c} \int_\Omega \theta \, \mathrm{d}\boldsymbol{x} = q_\alpha, \\ \lambda^-_{\theta(\boldsymbol{x})} \mathbf{I} \le \mathbf{A}(\boldsymbol{x}) \le \lambda^+_{\theta(\boldsymbol{x})} \mathbf{I}, \text{ a.e. } \boldsymbol{x} \end{array} \right\}$$

and with it

$$\text{(B)} \qquad \max_{(\theta,\mathbf{A})\in\mathcal{B}} J(\theta, \mathbf{A}) = \max_{(\theta,\mathbf{A})\in\mathcal{B}} \int_\Omega f u \, \mathrm{d}\boldsymbol{x}$$

Rewrite B as a max-min problem

Define $\mathcal{S} := \left\{\boldsymbol{\sigma} \in L^2(\Omega, \mathbb{R}^d),\ -\operatorname{div}(\boldsymbol{\sigma}) = f\right\}$

One can rewrite functional J in terms of fluxes:

$$J(\theta, \mathbf{A}) = \min_{\boldsymbol{\sigma}\in\mathcal{S}} \int_\Omega \mathbf{A}^{-1}\,\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}$$

With notation $\mathcal{C} = \left\{(\theta, \mathbf{A}) \,|\, (\theta, \mathbf{A}^{-1}) \in \mathcal{B}\right\}$

$$\begin{aligned}
\max_{(\theta,\mathbf{A})\in\mathcal{B}} J(\theta, \mathbf{A}) &= \max_{(\theta,\mathbf{A})\in\mathcal{B}} \min_{\boldsymbol{\sigma}\in\mathcal{S}} \int_\Omega \mathbf{A}^{-1}\,\boldsymbol{\sigma}\cdot\boldsymbol{\sigma} \\
&= \max_{(\theta,\mathbf{B})\in\mathcal{C}} \min_{\boldsymbol{\sigma}\in\mathcal{S}} \int_\Omega \mathbf{B}\,\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}
\end{aligned}$$

Conclusions

Next step is to apply theory of saddle points.
First, one can conclude that $\boldsymbol{\sigma}^*$ is unique.
Second, instead of solving convex problem B, one can solve the following optimization problem:

$$
\text{(I)} \qquad \begin{cases} I(\theta) = \int_\Omega f u \, \mathrm{d}x \to \max \\ s.t. \quad \theta \in L^\infty(\Omega, [0,1]), \ \int_\Omega \theta = q_\alpha, \ \text{where } u \text{ satisfies} \\ -\operatorname{div}(\lambda_\theta^- \nabla u) = f, \quad u \in \mathrm{H}_0^1(\Omega) \end{cases}
$$

Define $\psi := |\boldsymbol{\sigma}^*|^2$.

Lemma

The necessary and sufficient condition of optimality for solution θ^* of optimal design problem (I) *simplifies to the existence of a Lagrange multiplier $c \geq 0$ such that*

$$
(3) \qquad \begin{array}{lcl} \psi > c & \Rightarrow & \theta^* = 1\,, \\ \psi < c & \Rightarrow & \theta^* = 0\,. \end{array}
$$

Spherical symmetry

For spherically symmetric problem such that:

- $\Omega = R(\Omega)$ for any rotation R
- f is radial function

it can be proved that there exists radial solution θ_R^* of (I).

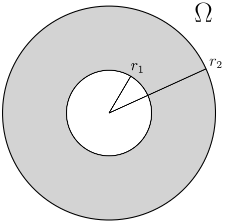
In particular, it can be shown that

$$\max_{(\theta,\mathbf{A})\in\mathcal{A}} J(\theta,\mathbf{A}) = I(\theta_R^*).$$

Design problems with spherical symmetry were studied for ball:

- **Single state equations**
  Murat & Tartar (1985) Calculus of Variations and Homogenization
  - there exists relaxed solution $(\theta^*, \mathbf{A}^*)$ among simple laminates.
- **Multiple state equations**
  Vrdoljak, M. (2016) Classical Optimal Design in Two-Phase Conductivity Problems. SIAM Journal on Control and Optimization: 2020-2035

Single state optimal design problem



$$\Omega = \overline{K}(0, r_2) \setminus K(0, r_1)$$

Single state equation:

$$(4) \qquad \begin{cases} -\operatorname{div}(\lambda_\theta^-(x)\nabla u) = 1 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

where $\lambda_\theta^-(x) = \left(\frac{\theta(x)}{\alpha} + \frac{1-\theta(x)}{\beta}\right)^{-1}$.

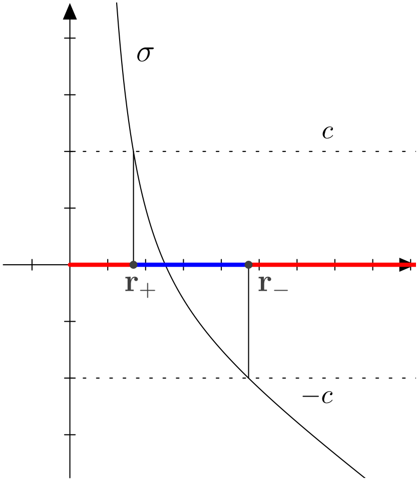
Optimization problem:

For $\theta \in \mathcal{T} := \left\{\theta \in L^\infty(\Omega, [0,1]) : \int_\Omega \theta \, d\boldsymbol{x} = q_\alpha\right\}$

$$I(\theta) = \int_\Omega u \, dx \to \max$$

One can rewrite (4) in polar coordinates :

$$-\frac{1}{r^{d-1}}(r^{d-1} \underbrace{\lambda_\theta^- u'(r)}_{\sigma})' = 1 \text{ in } \langle r_1, r_2\rangle\,, \quad u(r_1) = u(r_2) = 0.$$



The necessary and sufficient condition of optimality for θ^* states

$$\begin{aligned} |\sigma^*| > c \quad &\Rightarrow \quad \theta^* = 1\,, \\ |\sigma^*| < c \quad &\Rightarrow \quad \theta^* = 0\,. \end{aligned}$$

There are only three possible candidates for optimal design:

1) $\theta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_-\rangle \\ 1, & r \in [r_-, r_2] \end{cases}$

2) $\theta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_2\rangle \end{cases}$

3) $\theta^*(r) = \begin{cases} 0, & r \in [r_1, r_-\rangle \\ 1, & r \in [r_-, r_2\rangle \end{cases}$

Simplification to a non-linear system

Necessary and sufficient condition of optimality can also be expressed as a non-linear system (unknowns $\gamma, c, r_+ r_-$):

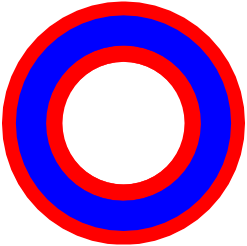
$$
(5) \qquad \begin{cases} S_d \int\limits_{r_1}^{r_2} \theta(\rho)\rho^{d-1}\,\mathrm{d}\rho = q_\alpha \\ u(r_2) = 0 \iff \gamma \int\limits_{r_1}^{r_2} \left(\frac{1}{a(\rho)\rho^{d-1}}\right)\mathrm{d}\rho = \int\limits_{r_1}^{r_2} \frac{\rho}{a(\rho)}\,\mathrm{d}\rho \\ \sigma(r_+) = c, \quad \sigma(r_-) = -c, \qquad \text{where } c > 0 \end{cases}
$$

where

$$
\sigma(r) = \frac{\gamma}{r^{d-1}} - \frac{r}{d}, \quad \& \quad a(r) = \left(\frac{\theta(r)}{\alpha} + \frac{1-\theta(r)}{\beta}\right)^{-1}.
$$

With this you can easily calculate the shape of domain.

Analytical solution:
$f = 1$, domain Ω is annulus and amount q_α is not scarce one can prove that shape design $\alpha - \beta - \alpha$ is optimal solution.



Remark:

- Problem can be generalized to multi-state problem where functional is given with $J(\chi) = \sum_{i=1}^m \mu_i \int_\Omega f_i u_i$.
- Existence of such solutions is important for any numerical method like shape derivative method.

Shape derivative

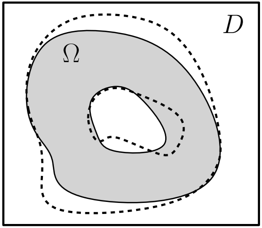
Perturbation of the set Ω is given with

$$\Omega_t = (\mathrm{Id} + t\psi)\Omega$$

where $\psi \in W^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d)$

This allows us to define shape derivative:

If t is small (i.e. $\|t\psi\|_{W^{k,\infty}} \ll 1$) mapping $\mathrm{Id} + t\psi$ is homeomorphism.



Definition (Shape derivative)

Let $J = J(\Omega)$ be a shape functional. J is said to be shape differentiable at Ω in direction ψ if

$$J'(\Omega, \psi) := \lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t}$$

exists and the mapping $\psi \mapsto J'(\Omega, \psi)$ is linear and continuous.
$J'(\Omega, \psi)$ is called the **shape derivative**.

Single state problem (general f)

For optimal design problem:

$$(\mathrm{P}) \qquad \begin{cases} J(\chi) = \int_\Omega f u \,\mathrm{d}\boldsymbol{x} \to \max \\ \text{s.t.} \quad \chi \in L^\infty(\Omega, \{0,1\}), \quad \int_\Omega \chi \,\mathrm{d}\boldsymbol{x} = q_\alpha, \\ u \text{ solves (1) with } \mathbf{A} = \chi\alpha\,\mathbf{I} + (1-\chi)\beta\,\mathbf{I}. \end{cases}$$

shape derivative is given with:

$$\begin{aligned} J'(\Omega,\psi) &= \int_\Omega \mathbf{A}(-\operatorname{div}(\psi) + \nabla\psi + \nabla\psi^\tau)\nabla u_0 \cdot \nabla u_0 \,\mathrm{d}\boldsymbol{x} \\ &+ \int_\Omega 2(\operatorname{div}(\psi) f + \nabla f \cdot \psi) u_0 \,\mathrm{d}\boldsymbol{x} \end{aligned}$$

where u_0 is solution of BVP (1) on domain Ω with $\mathbf{A}$.

Lagrangian method using shape derivative

Choice of vector field ψ:
Vector field $\psi \in H_0^1(\Omega)$ can be constructed from variational formulation:

$$\int_\Omega \nabla\psi : \nabla\varphi + \int_\Omega \psi \cdot \varphi = J'(\Omega, \varphi), \quad \forall \varphi \in H_0^1(\Omega)$$

With this approach regularity of ψ is higher than usual (L^2) which is particularly good regardless the method.
Observe that thus created ψ is ascent direction for our problem because

$$J(\Omega_t) = J(\Omega) + tJ'(\Omega, \psi) + o(t)$$

and

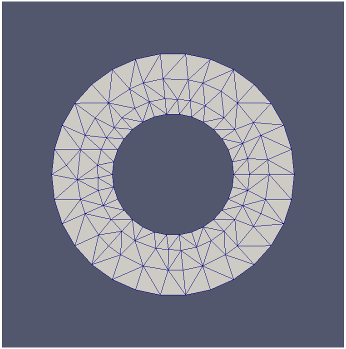
$$J'(\Omega, \psi) = \|\psi\|_{H^1}^2 > 0 \text{ (by construction)}$$

Lagrangian method using shape derivative

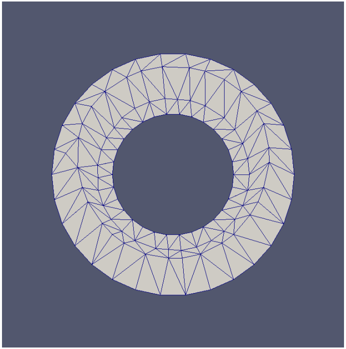
It is important to note:

- outer boundaries stays the same
- only boundary between phases is changing.

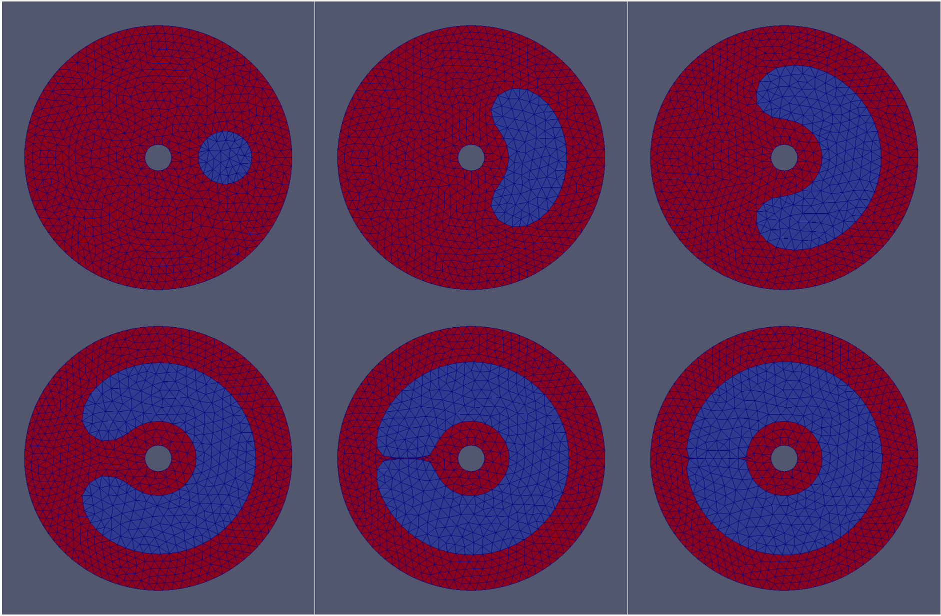
This is implemented using `movemesh` from freefem++.
Remeshing is necessary with this approach.



$\Rightarrow$
one step ϕ_t



Numerical results - simple connected set



Numerical results