Optimal coefficients for elliptic PDEs

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X Partial Differential Equations, Optimal Design and Numerics

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For a fixed bounded domain Ω and right-hand side f let u_a be the unique solution of the elliptic PDE

$$\begin{cases} -\operatorname{div}(a\nabla u) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

Given a class $\mathcal{A}$ of admissible choices we want to solve an optimization problem of the form

$$\min\Big\{\int_\Omega j(x, u_a)\,dx \ :\ a \in \mathcal{A}\Big\}.$$

Joint work with M.S. Gelli and D. Lučić (SIAM Math. Anal. 2023)

This is an optimal control problem, with state variable u, control variable a, state equation

$$\begin{cases} -\,\mathrm{div}(a\nabla u) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

and cost functional

$$J(u) = \int_\Omega j(x,u)\,dx.$$

The space of states is the Sobolev space $H_0^1(\Omega)$ and the class of admissible controls is $\mathcal{A}$.

This is part of a larger research program, with J. Casado-Díaz and F. Maestre (U. Sevilla), concerning optimization problems for elliptic PDEs, where one is interested in:

- optimal coefficients for $-\operatorname{div}\left(a(x)\nabla u\right) = f$;
- optimal potentials for $-\Delta u + V(x)u = f$;
- optimal right-hand side for $-\Delta u = f$.

In this lecture we focus on the first problem.

The simplest case is when $j(x,s) = f(x)s$, that is we want to minimize the quantity (called compliance)

$$\mathcal{C}(a) = \int_\Omega f(x) u_a \, dx.$$

This corresponds to determine the density of material producing the stiffest membrane (for a given load f). By an integration by parts we easily find that $\mathcal{C}(a) = -2\mathcal{E}(a)$, where $\mathcal{E}$ is the energy

$$\mathcal{E}(a) = \inf \left\{ \int_\Omega \left(\frac{a(x)}{2} |\nabla u|^2 - f(x) u \right) dx \ : \ u \in C_0^1(\Omega) \right\}.$$

If the admissible class is of the form

$$\mathcal{A} = \left\{ \int_\Omega \psi(a)\, dx = m \right\},$$

with ψ convex, by a Lagrange multiplier λ (no loss of generality for taking $\lambda = 1$) we are reduced to the problem

$$\inf \left\{ \mathcal{C}(a) + \int_\Omega \psi(a)\, dx \ : \ a \geq 0 \right\},$$

or equivalently (recall that $\mathcal{C}(a) = -2\mathcal{E}(a)$)

$$\sup \left\{ \mathcal{E}(a) - \frac{1}{2} \int_\Omega \psi(a)\, dx \ : \ a \geq 0 \right\}.$$

This is a max / min problem:

$$\sup_{a\geq 0}\left\{\inf_{u=0 \text{ on } \partial\Omega}\int_\Omega\left(\frac{1}{2}a|\nabla u|^2 - f(x)u - \frac{1}{2}\psi(a)\right)dx\right\}.$$

Assume first ψ is superlinear, that is:

$$\lim_{s\to+\infty}\frac{\psi(s)}{s} = +\infty.$$

Theorem. *In this case there exists an optimal coefficient* $a_{opt} \in L^1(\Omega)$.

The proof easily follows by the direct methods of the calculus of variations.

Indeed, for every $u \in C_0^1(\Omega)$ the map

$$a \mapsto \int_\Omega \left(\frac{1}{2}a(x)|\nabla u|^2 - f(x)u - \frac{1}{2}\psi(a)\right) dx$$

is weakly $L^1(\Omega)$ upper semicontinuous. Then $\mathcal{E}(a)$ (infimum of a family of upper semicontinuous functions) is weakly $L^1(\Omega)$ upper semicontinuous too. In addition, testing with $u = 0$, we have $\mathcal{E}(a) \leq 0$ and we obtain

$$\int_\Omega \psi(a)\, dx \leq C.$$

Then, by the superlinearity of ψ, the existence of an optimal coefficient $a_{opt} \in L^1(\Omega)$ is easily established.

We want now to characterize the optimal coefficients a_{opt} by means of some suitable auxiliary variational problem.

It is well known that in general $\sup_A \inf_B$ is different from $\inf_B \sup_A$, but the case above is very particular, with the function of the pair (a, u) convex with respect to the variable u and concave with respect to the variable a. Thanks to a result from min/max theory [Ekeland 1975] we may exchange the order of inf and sup.

We then obtain the optimization problem

$$\inf_{u \in C_0^1(\Omega)} \left\{ \sup_{a \geq 0} \int_\Omega \left(\frac{1}{2} a |\nabla u|^2 - f(x) u - \frac{1}{2} \psi(a) \right) dx \right\}.$$

The supremum with respect to the variable a can now be easily computed:

$$\sup_{a \geq 0} \int_\Omega \left(\frac{1}{2} a(x) |\nabla u|^2 - f(x) u - \frac{1}{2} \psi(a) \right) dx$$
$$= \int_\Omega \left(\frac{1}{2} \psi^* \left(|\nabla u|^2 \right) - f(x) u \right) dx,$$

where ψ^* is the Legendre-Fenchel conjugate function of ψ, given by

$$\psi^*(t) = \sup \left\{ st - \psi(s) \ : \ s \geq 0 \right\}.$$

The auxiliary variational problem is then

$$\inf_{u \in C_0^1(\Omega)} \int_\Omega \left(\frac{1}{2} \psi^* \left(|\nabla u|^2 \right) - f(x) u \right) dx.$$

We then proceed in the following way:

Step 1. Solve the auxiliary variational problem and get its solution $\bar{u}$, that belongs to $H_0^1(\Omega)$, since the coercivity comes from the inequality

$$\psi^*(t) \geq t - \psi(1).$$

Step 2. Recover the optimal coefficient a_{opt} by the necessary conditions of optimality

$$a_{opt}|\nabla \bar{u}|^2 = \psi(a_{opt}) + \psi^*(|\nabla \bar{u}|^2).$$

For instance, if $\psi(s) = s^2/2$ we obtain the auxiliary variational problem

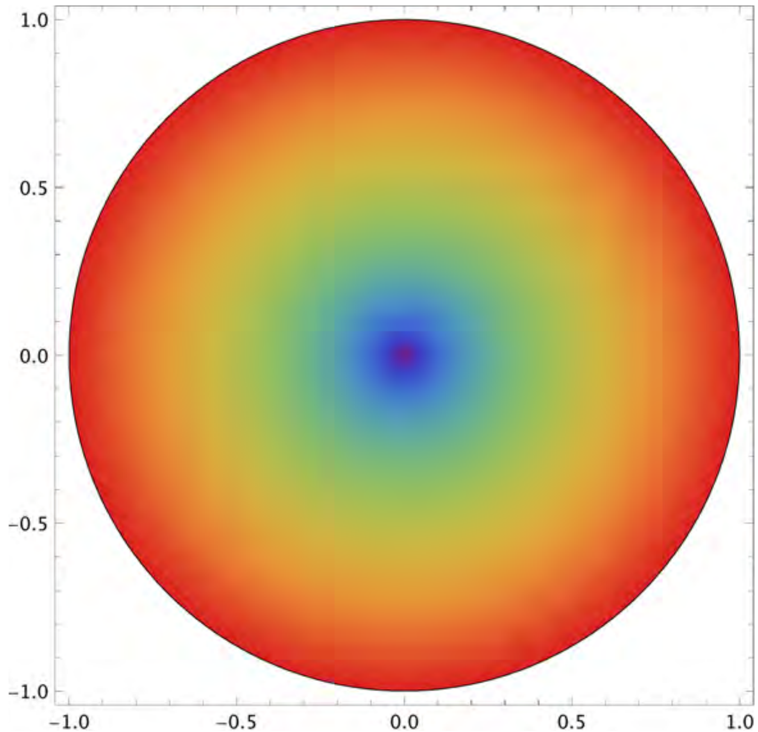
$$\min \left\{ \int_\Omega \left(\frac{1}{4}|\nabla u|^4 - f(x)u \right) dx \ : \ u \in H_0^1(\Omega) \right\},$$

or equivalently the nonlinear PDE

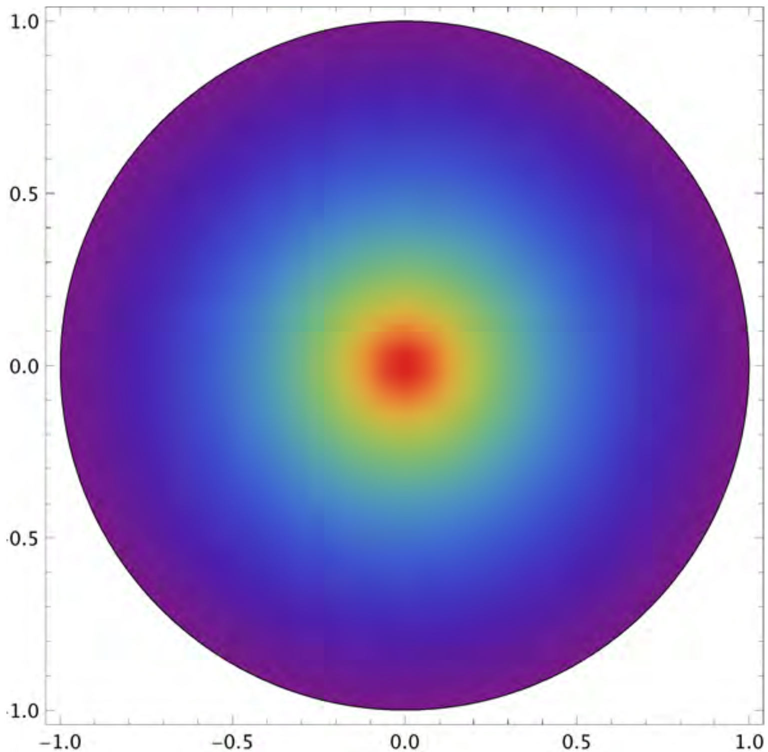
$$-\Delta_4 u = f, \qquad u \in W_0^{1,4}(\Omega),$$

whose unique solution $\bar{u}$ provides the optimal coefficient $a_{opt}(x) = |\nabla \bar{u}(x)|^2$.

If Ω is the unit disk in $\mathbf{R}^2$ and $f = 1$ this gives $a_{opt}(x) = (|x|/2)^{2/3}$.



If Ω is the unit disk in $\mathbf{R}^2$ and $f = \delta_0$ this gives $a_{opt}(x) = (2\pi|x|)^{-2/3}$.



Another interesting case is when some a priori bounds on the admissible coefficients a are imposed, that is

$$\psi(s) = \begin{cases} s & \text{if } s \in [\alpha, \beta] \\ +\infty & \text{otherwise,} \end{cases}$$

with $0 \leq \alpha < \beta$. Computing the conjugate function ψ^* gives the auxiliary variational problem

$$\min_{u \in H_0^1(\Omega)} \left\{ \int_\Omega \left(\frac{|\nabla u|^2 - 1}{2} \left[\beta 1_{\{|\nabla u| > 1\}} + \alpha 1_{\{|\nabla u| \leq 1\}} \right] - f(x) u \right) dx \right\}.$$

By strict convexity, the auxiliary variational problem above admits a unique solution $\bar{u}$.

We then obtain the necessary conditions of optimality

$$\begin{cases} a_{opt} = \beta & \text{if } |\nabla \bar{u}| > 1 \\ a_{opt} = \alpha & \text{if } |\nabla \bar{u}| < 1 \\ a_{opt} \in [\alpha, \beta] & \text{if } |\nabla \bar{u}| = 1. \end{cases}$$

The case when ψ has only a linear growth:

$$\lim_{s \to +\infty} \frac{\psi(s)}{s} = k > 0,$$

is more delicate. In fact, denoting by $\mathcal{M}(\Omega)$ the class of nonnegative measures in Ω, the existence result is the following.

Theorem. *In this case there exists an optimal coefficient $a_{opt} \in \mathcal{M}(\Omega)$.*

The proof is similar to the previous one, by the direct methods of the calculus of variations with the weak convergence of measures.

In some situations it is important to allow the right-hand side f to be singular, for instance with concentrations on regions of lower dimensions.

For a measure μ the energy $E(\mu)$ can be still defined as an infimum:

$$\mathcal{E}(\mu) = \inf \left\{ \frac{1}{2} \int |\nabla u|^2 \, d\mu - \int_\Omega u \, df \ : \ u \in C_0^1(\Omega) \right\}.$$

The definition of the convex term $\int \psi(\mu)$, is well-known and amounts to

$$\int \psi(\mu) = \int_\Omega \psi(\mu^0) \, dx + k|\mu^s|,$$

where $\mu = \mu^0 \, dx + \mu^s$ is the Radon-Nikodym decomposition of μ into absolutely continuous and singular parts (with respect to the Lebesgue measure), $|\mu^s|$ is the *total variation* of the singular measure μ^s, and k is the so-called *recession coefficient*.

Therefore, if $\mathcal{M}$ is the class of nonnegative measures, the compliance optimization problem has still the form

$$\sup_{\mu \in \mathcal{M}} \inf_{u \in C_0^1(\Omega)} \int \frac{1}{2} |\nabla u|^2 \, d\mu - \int u \, df - \int \frac{1}{2} \psi(\mu).$$

The question is to see what is the PDE corresponding to a measure μ, or equivalently, what is a more explicit way of writing the energy $\mathcal{E}(\mu)$. This problem was considered by [Bouchitté-B. 2001], where the notion of *tangential gradient* $\nabla_\mu u$ was introduced.

This allows to define the Sobolev space $H^1_{0,\mu}$ as the closure of $C^1_0(\Omega)$ with respect to the norm

$$\Big(\int |\nabla_\mu u|^2\,d\mu + \int_\Omega u^2\,dx\Big)^{1/2}.$$

The optimal compliance problem then takes the form

$$\max_{\mu\in\mathcal{M}} \min_{u\in H^1_{0,\mu}} \int \frac{1}{2}|\nabla_\mu u|^2\,d\mu - \int u\,df - \int \frac{1}{2}\psi(\mu).$$

The most studied case is when $\psi(s)$ is linear, which corresponds to find the stiffest structure for the datum f, under a constraint on the total mass of the measure μ, that we take equal to 1 for simplicity. This give raise to the PDE

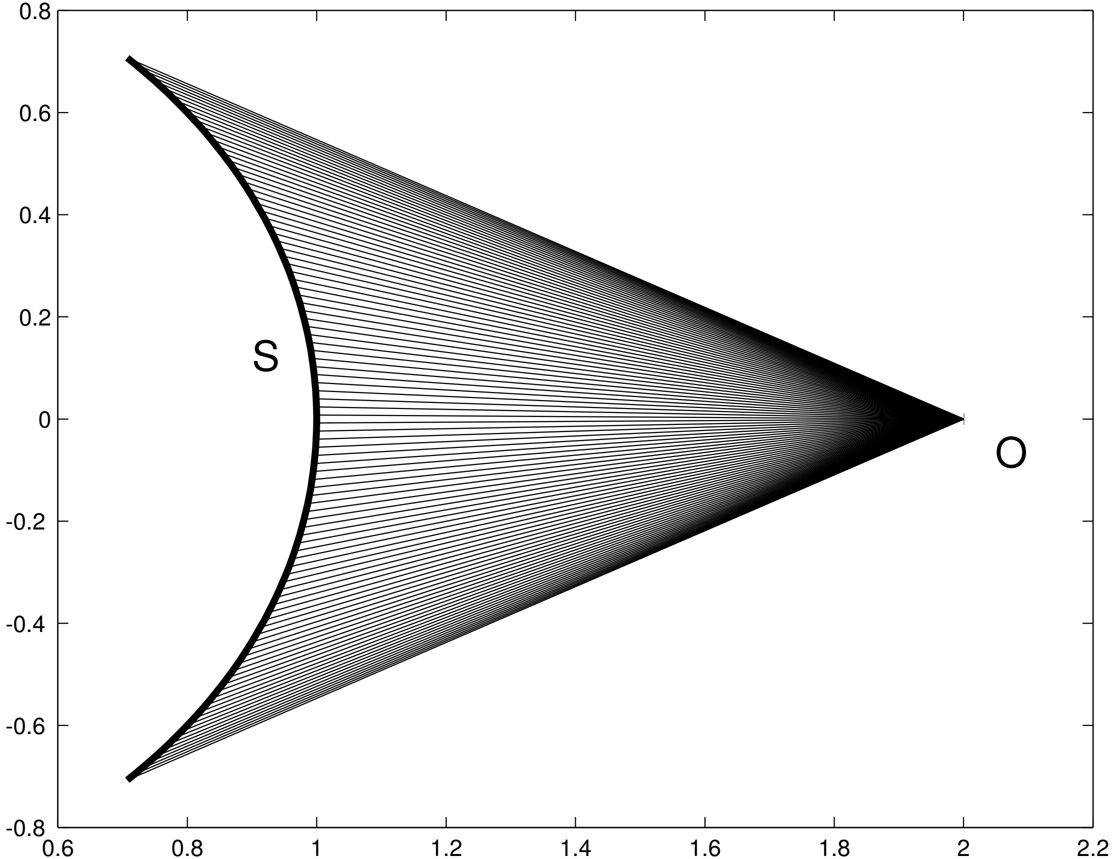
$$\begin{cases} -\,\mathrm{div}(\mu\nabla_\mu u) = f \\ |\nabla u| \le 1 \text{ and } |\nabla_\mu u| = 1\ \mu\text{-a.e.} \end{cases}$$

where μ is a probability measure on Ω and u is a Lipschitz function vanishing on $\partial\Omega$ (or simply a Lipschitz function in the Neumann case, when the right-hand side f has zero average).

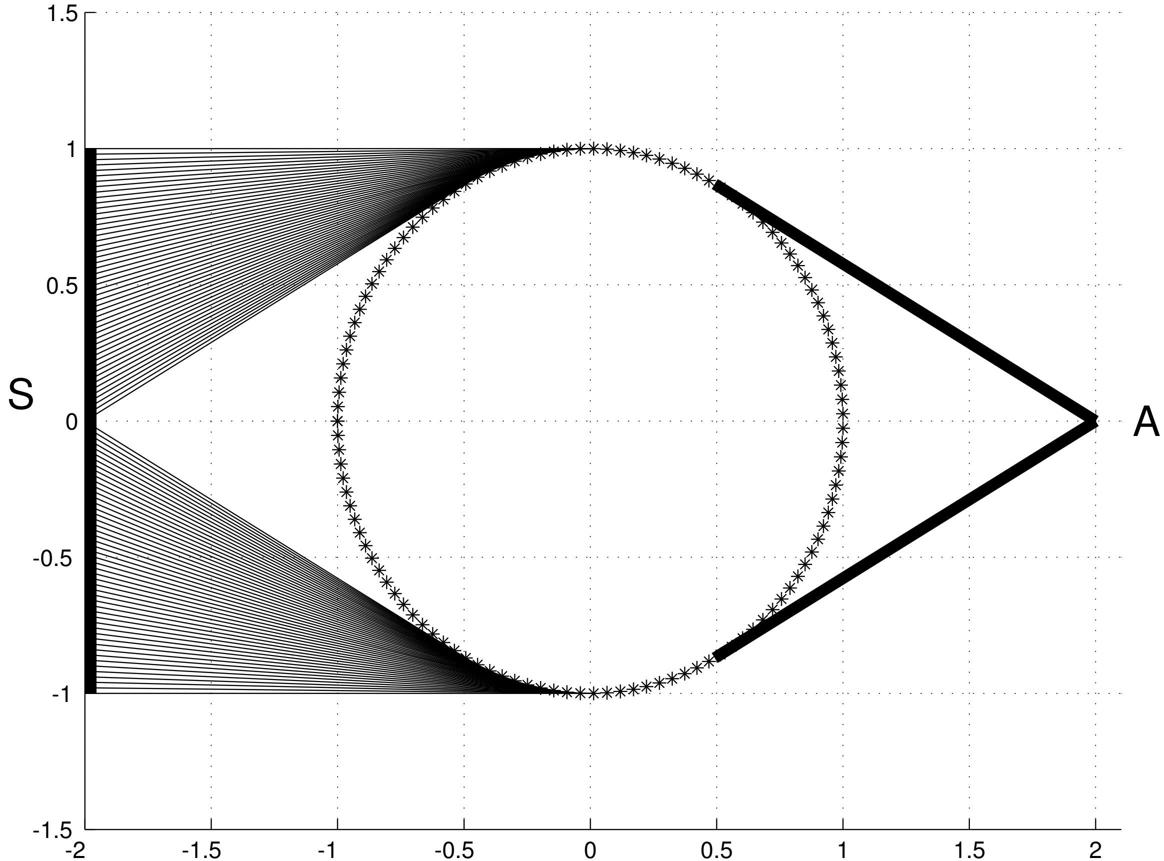
This is exactly the Monge-Kantorovich equation that comes from optimal transport theory; in other words, when $\psi(s) = s$ the problem of optimal coefficients is equivalent to an optimal transport problem.

The optimal measure μ is called in transport theory *transport density* and describes the density of transport trajectories that bring in an optimal way, for the transport cost $|x-y|$, the positive part f^+ onto the negative part f^- (in the Neumann case), or the source f on $\partial\Omega$ (in the Dirichlet case).

For instance, the following figure represents the optimal mass density for the Neumann problem, when the source f is a positive Dirac mass at the point O and a negative mass uniformly distributed on the curve S of unitary length.



Optimal mass density for the compliance problem.



Optimal mass density with an obstacle.

There is a very wide literature on optimal transport problems, we recall here the main facts about the measure μ_{opt}.

$$f \in \mathcal{M} \implies \mu_{opt} \in \mathcal{M} \text{ possibly not unique;}$$

$$f \in L^1(\Omega) \implies \mu_{opt} \in L^1(\Omega) \text{ and is unique;}$$

$$f \in L^p(\Omega) \implies \mu_{opt} \in L^p(\Omega) \text{ for every } p \in [1, +\infty];$$

$$\text{spt}(\mu_{opt}) \subset \text{convex envelope of } \begin{cases} \text{spt}(f) \text{ (Neumann)} \\ \text{spt}(f) \cup \partial\Omega \text{ (Dirichlet)} \end{cases}$$

In addition, a mild BV and $W^{1,1}$ regularity for μ_{opt} is available in dimension two, in some particular cases.

More precisely, when $d = 2$, under some regularity assumptions on Ω, and for some particular cases of f, we have ([Dweik 2024]):

$$f \in BV(\Omega) \cap L^\infty(\Omega) \quad \Longrightarrow \quad \mu_{opt} \in BV(\Omega),$$
$$f \in W^{1,1}(\Omega) \cap L^\infty(\Omega) \quad \Longrightarrow \quad \mu_{opt} \in W^{1,1}(\Omega).$$

As far as we know, no regularity results are available in higher dimension.

Furthermore, the correspondence between the optimization and transport problems is unclear when the function ψ is nonlinear.

An optimization problem more general than the minimal compliance is the one written in a control form:

$$\min\left\{ \int_\Omega \Big(j(x,u_a)+\psi(a)\Big)\,dx \ :\ a\ge 0\right\},$$

where u_a solves the PDE

$$-\operatorname{div}\Big(a(x)\nabla u\Big)=f,\qquad u=0 \text{ on } \partial\Omega.$$

In this case the equivalence with an optimal transport problem is lost and the existence of an optimal coefficient fails in general.

Some counterexamples are available:

- [Murat 1977] with $j(x,s) = |s - u_0(x)|^2$, $f = 0$, but with a boundary datum $u = g$ on $\partial\Omega$.

- [B.-Casado Diaz-Maestre 2024] with $j(x,s) = h(x)s$, $f = 1$, and $u = 0$ on $\partial\Omega$.

In these cases we need to relax the problem in order to study the asymptotic behavior of minimizing sequences.

It is known [Murat-Tartar 1985] that a sequence a_n of coefficients between two positive constants α and β may tend (in the sense of convergence of the corresponding solutions, the G-convergence introduced in 1973 by De Giorgi and Spagnolo) to a symmetric $d \times d$ matrix $A(x)$.

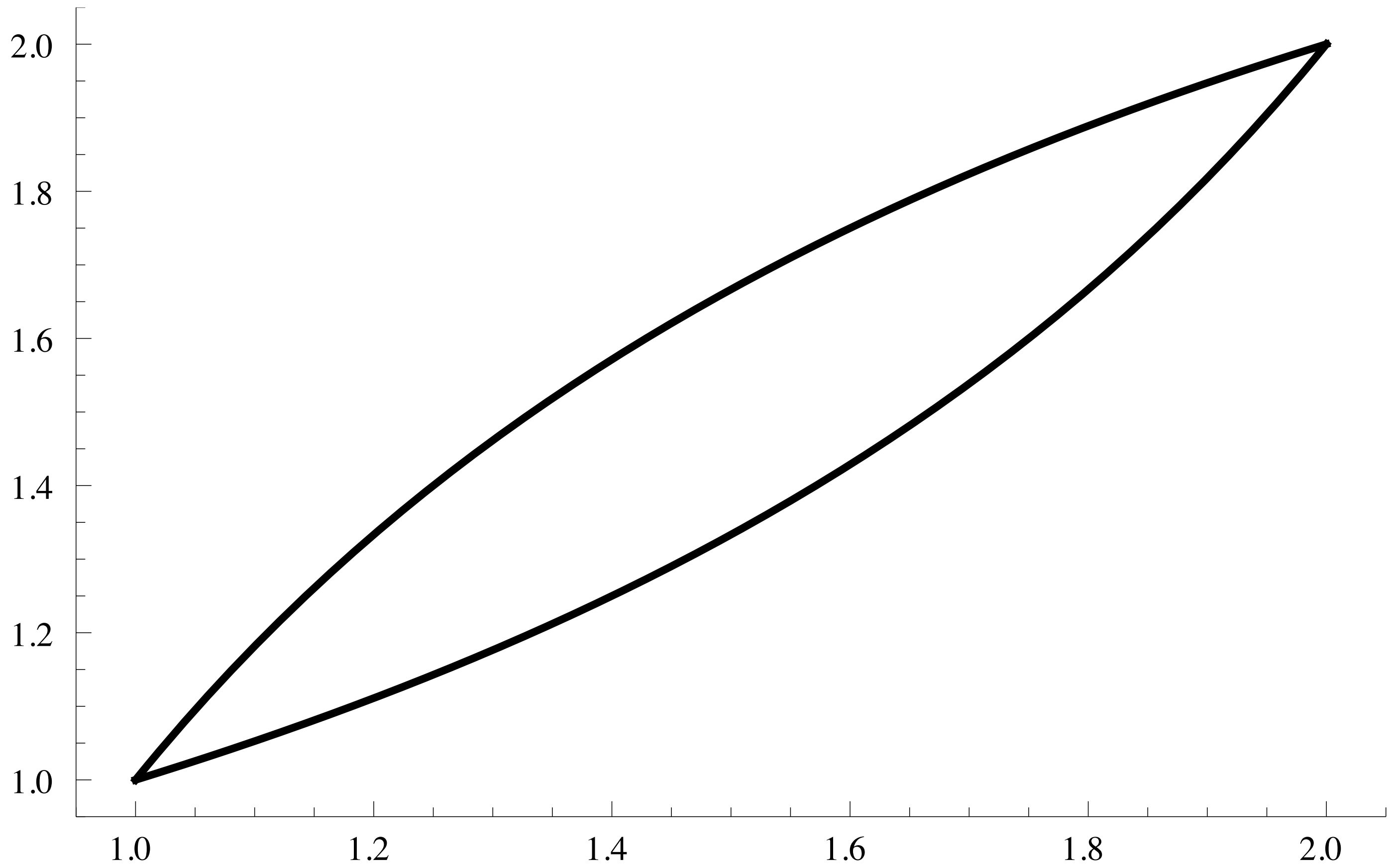
The set $M(\alpha, \beta)$ of all the matrices A attainable in this way is completely characterized in terms of some inequalities that have to be satisfied by their eigenvalues.

For instance, when $d = 2$, the set above is given by the symmetric 2×2 matrices $A(x)$ whose eigenvalues $\lambda_1(x)$ and $\lambda_2(x)$ are between α and β and satisfy the inequalities

$$\frac{\alpha\beta}{\alpha + \beta - \lambda_1(x)} \leq \lambda_2(x) \leq \alpha + \beta - \frac{\alpha\beta}{\lambda_1(x)} \, .$$

In the following figure we plot the set of attainable symmetric matrices A, in the plane (λ_1, λ_2) of eigenvalues, when

$$\alpha = 1, \qquad \beta = 2.$$



Region for eigenvalues of attainable matrices.

The relaxation of the control problem above has been studied when the penalization function ψ is linear [Cabib-Dal Maso 1988]. The optimal control problem

$$\min\left\{\int_\Omega \Big(j(x,u_a)+a\Big)\,dx\ :\ \alpha\le a\le\beta\right\},$$

admits the relaxed formulation

$$\min\left\{\int_\Omega \Big(j(x,u_A)+\lambda_d\big(A(x)\big)\Big)\,dx\ :\ A\in M(\alpha,\beta)\right\},$$

where $\lambda_d(A)$ is the largest eigenvalue of A.

No regularity results, similar to the compliance case, are available.

In order to illustrate numerically the nonexistence example above, we take in $\mathbf{R}^2$ the unitary ball B and the PDE

$$\begin{cases} -\operatorname{div}\Big(a(x)\nabla u\Big) = 1 \quad \text{in } B \\ u \in H_0^1(B). \end{cases}$$

The coefficient $a(x)$ has to be chosen to minimize the cost

$$\int_B (1+\varepsilon x_1) u \, dx + \frac{1}{2}\int_B a(x)\, dx$$

under the constraint $a(x) \in [1,2]$. If $\varepsilon = 0$ we have the minimal compliance problem, that admits an optimal coefficient $a(x)$.

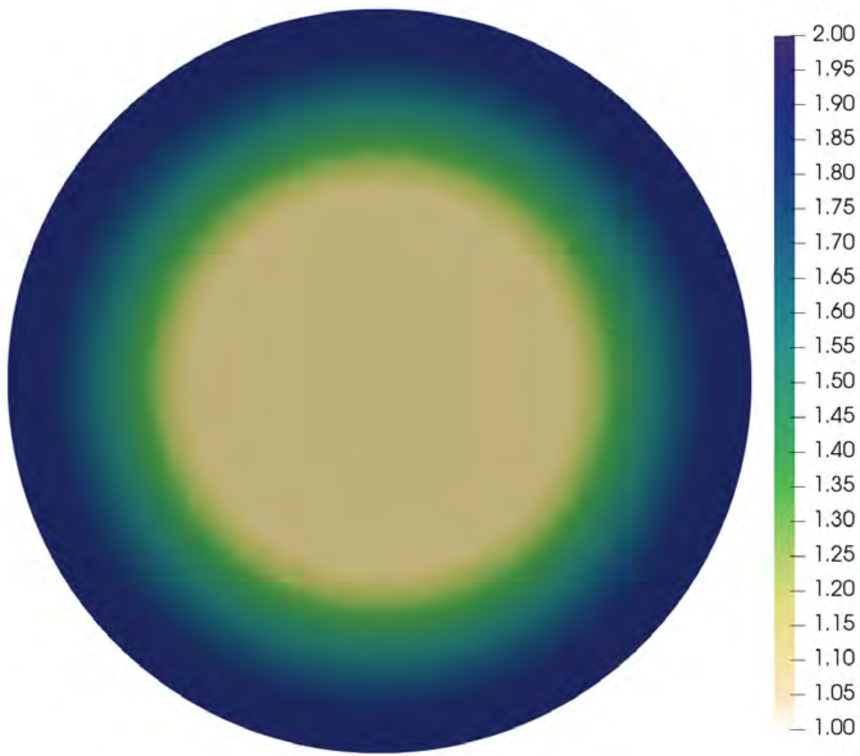
When $\varepsilon > 0$ on the contrary we have seen that no optimal coefficient exists and the problem has to be relaxed obtaining 2×2 symmetric matrices $A(x)$ that optimize the cost

$$\int_B (1 + \varepsilon x_1) u \, dx + \frac{1}{2} \int_B \lambda_{max}(x) \, dx,$$

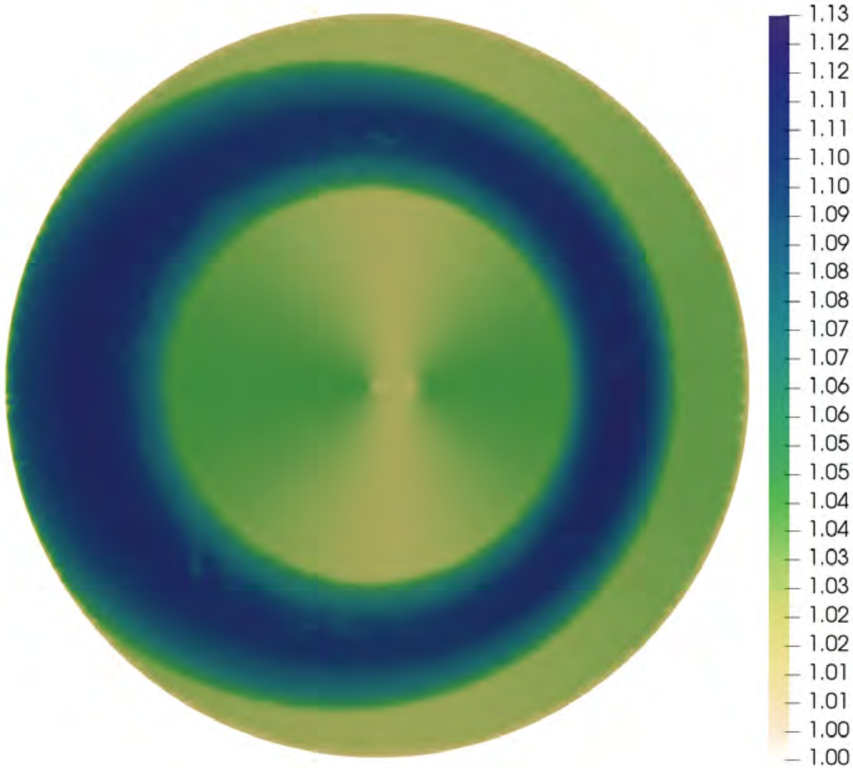
where λ_{max} is the largest eigenvalue of $A(x)$ and u solves

$$\begin{cases} -\operatorname{div}\Big(A(x)\nabla u\Big) = 1 & \text{in } B \\ u \in H_0^1(B). \end{cases}$$

We plot below the two cases.



For $\varepsilon = 0$ the optimal coefficient $a(x)$ exists and is represented above.



For $\varepsilon = 0.5$ we plot the ratio $\lambda_{max}/\lambda_{min}$ of the optimal matrix $A(x)$.

In structural mechanics problems one looks for the stiffest elastic structure, the appropriate framework is linear elasticity; the function $u : \Omega \to \mathbf{R}^d$ is vector valued, the load f is a vector measure in Ω, and the energy $\mathcal{E}(a)$ is

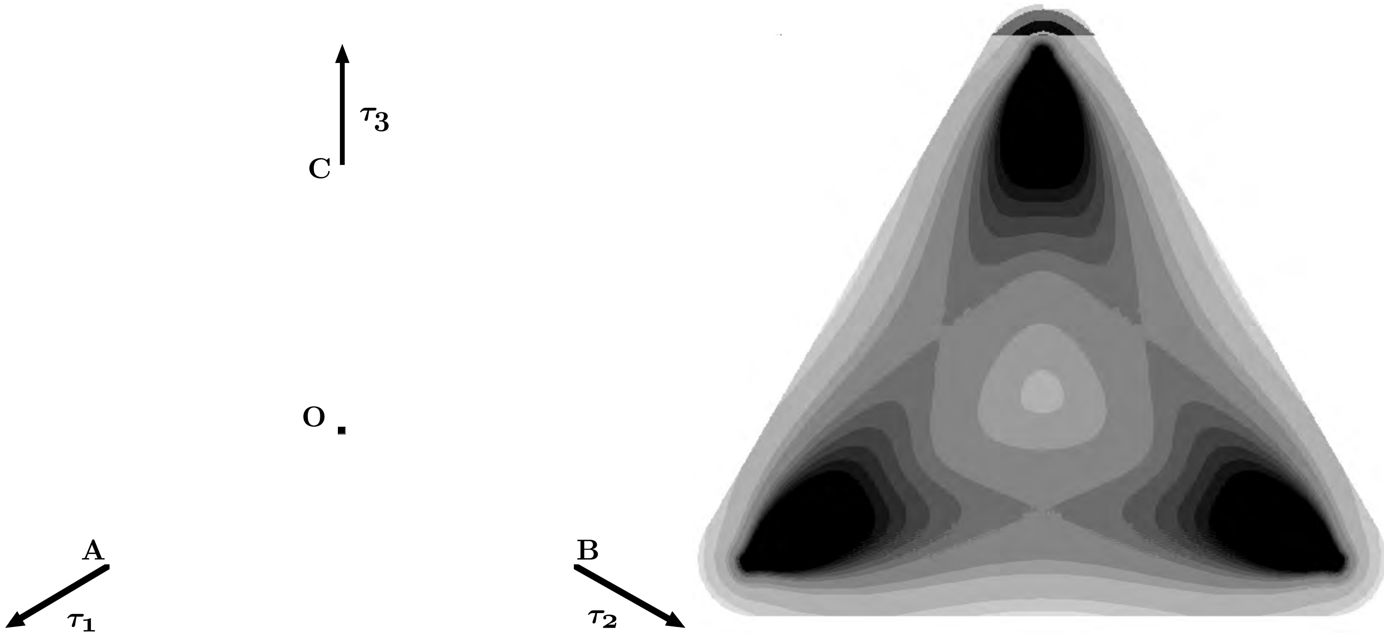
$$\mathcal{E}(a) = \inf \left\{ \int_\Omega \left(\frac{1}{2} a(x) j(\nabla u) - f(x) u \right) dx \right\}$$

with $u \in H_0^1(\Omega; \mathbf{R}^d)$ in the Dirichlet case, or $u \in H^1(\Omega)$ in the Neumann case, where j is the quadratic form of linear elasticity on symmetric $d \times d$ matrices, involving the Lamé constants of the material.

The minimal compliance problem is then similarly written as before, with $\mathcal{C}(a) = -2\mathcal{E}(a)$, but the connection with some form of transport problem is missed and some differences with respect to the scalar case are known. The existence of an optimal measure μ_{opt} can still be obtained in a similar way as before, but the property that

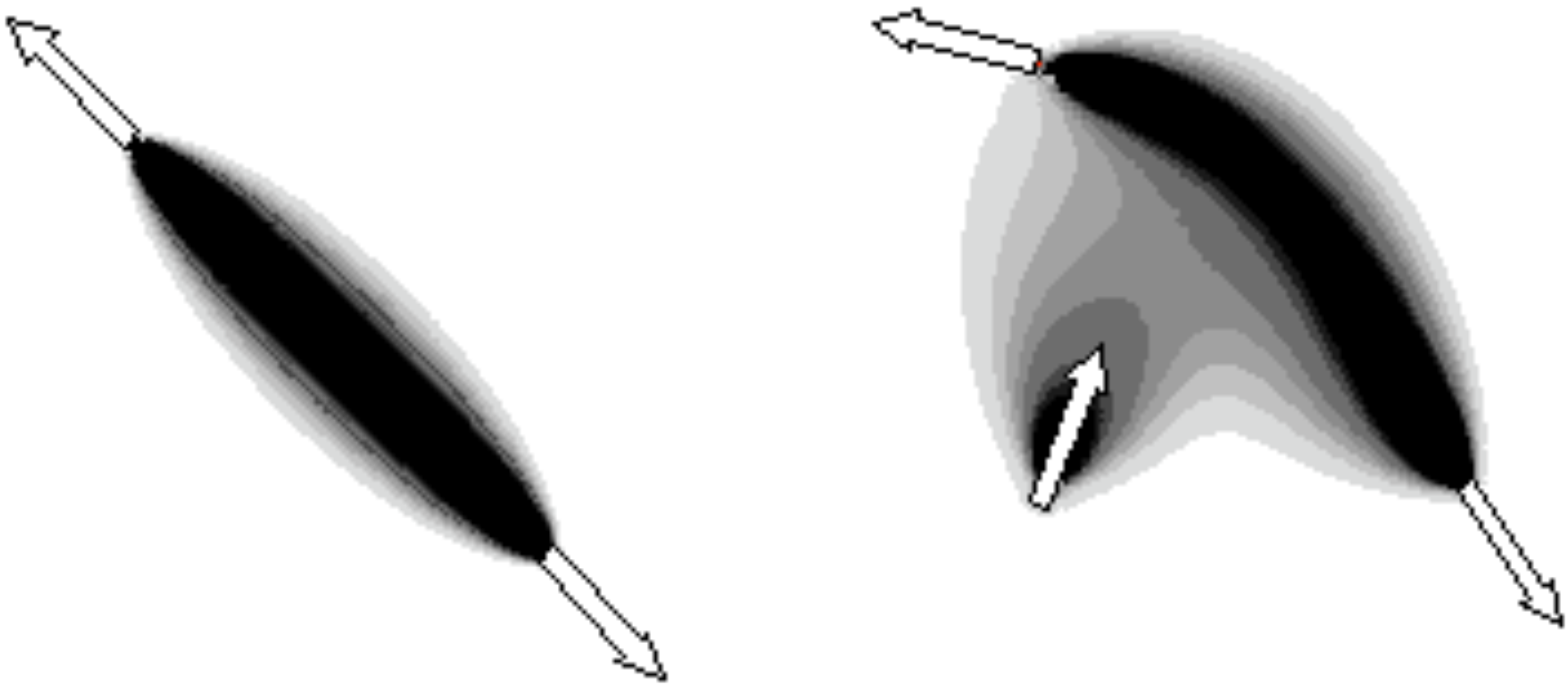
$$\text{spt}(\mu_{opt}) \subset \text{convex envelope of spt}(f)$$

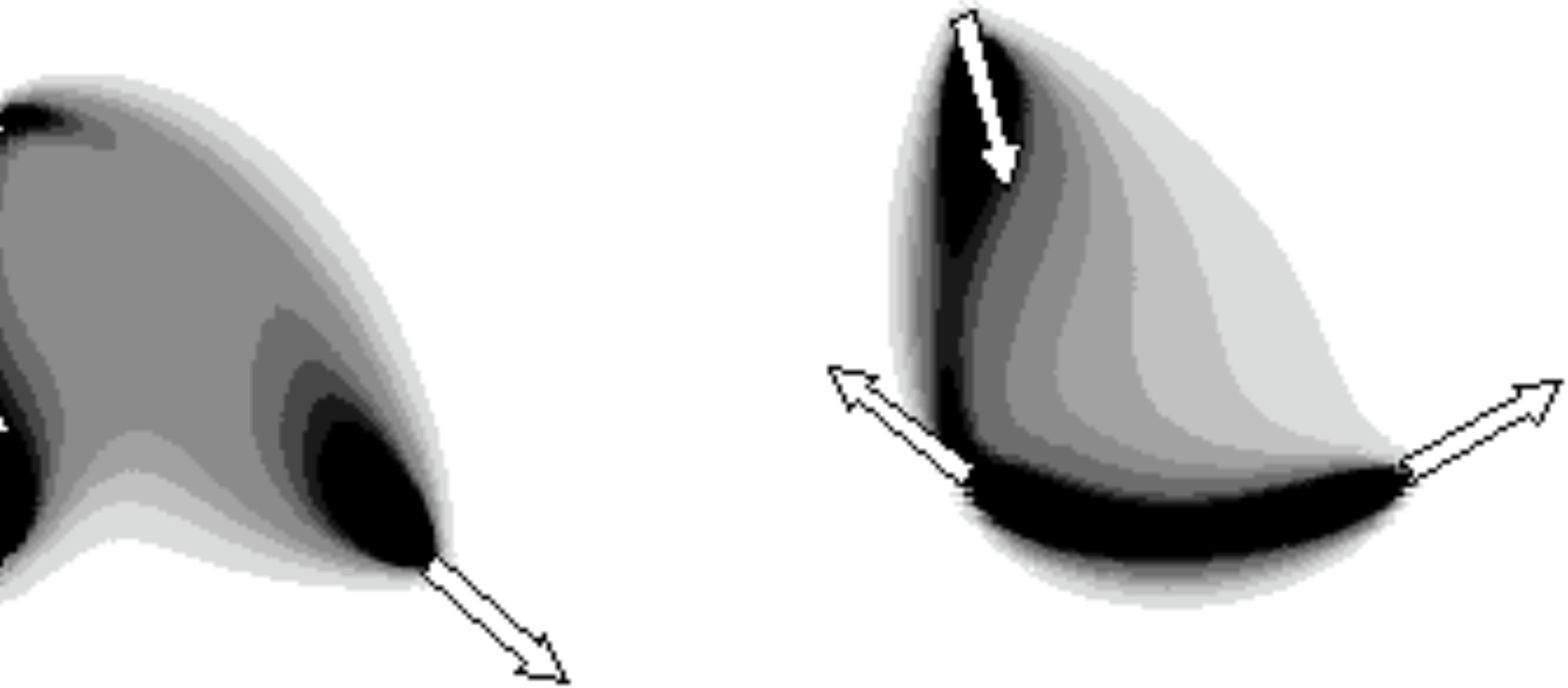
is no longer true as the two-dimensional example below shows.

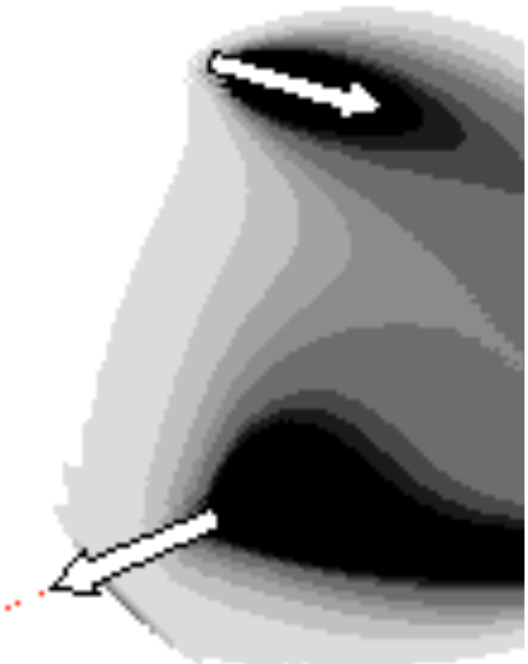


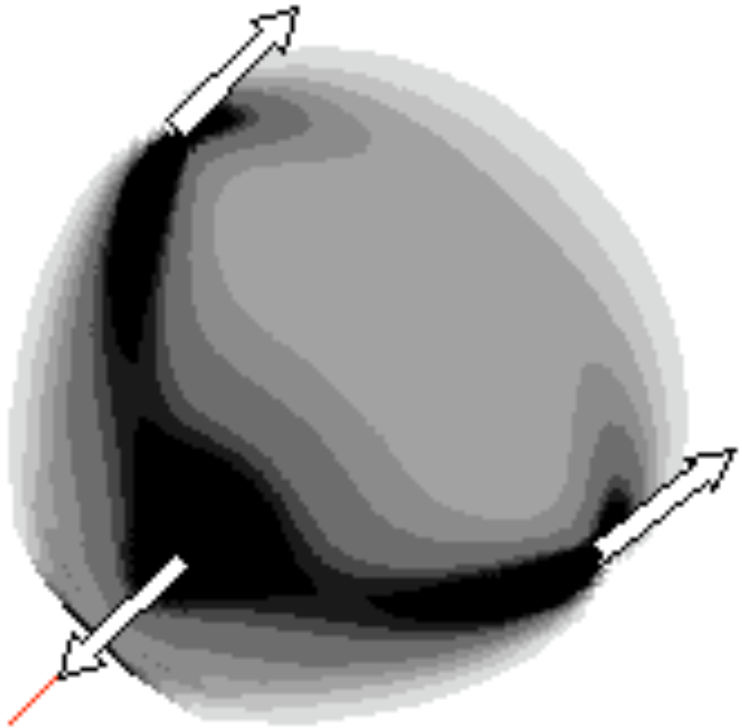
The force field f (left) and the optimal density μ_{opt} (right).

sent in an optimal design.









This conjecture, if

Thanks for your attention