



Variant of Optimality Criteria Method for Multiple State Optimal Design Problems

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Stationary diffusion equation

Let $\Omega \subseteq \mathbf{R}^d$ be open and bounded, $\mathbf{A} = \mathbf{A}^\top \in L^\infty(\Omega; \mathcal{M}_{\alpha,\beta})$,

$$\mathcal{M}_{\alpha,\beta} := \left\{ \mathbf{A} \in \mathbf{M}_d(\mathbf{R}) : (\forall \xi \in \mathbf{R}^d) \quad \mathbf{A}\xi \cdot \xi \geq \alpha|\xi|^2, \mathbf{A}^{-1}\xi \cdot \xi \geq \frac{1}{\beta}|\xi|^2 \right\}$$

and $f \in H^{-1}(\Omega)$. Stationary diffusion equation with homogenous Dirichlet boundary condition:

$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla u) = f \\ u \in H_0^1(\Omega) \end{cases}$$

Ω - mixture of two isotropic materials with conductivities $0 < \alpha < \beta$:

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

where $\chi \in L^\infty(\Omega; \{0, 1\})$.



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Optimal design problem (single state)

$$\begin{cases} J(\chi) = \int_{\Omega} [\chi(\mathbf{x})g_{\alpha}(\mathbf{x}, u(\mathbf{x})) + (1 - \chi(\mathbf{x}))g_{\beta}(\mathbf{x}, u(\mathbf{x}))] d\mathbf{x} \longrightarrow \min, \\ \chi \in L^{\infty}(\Omega; \{0, 1\}), \int_{\Omega} \chi d\mathbf{x} = q_{\alpha}, \end{cases}$$

where $\Omega \subseteq \mathbf{R}^d$ open and bounded, $f \in H^{-1}(\Omega)$, $0 < \alpha < \beta$, $0 < q_{\alpha} < |\Omega|$, and g_{α}, g_{β} Caratheodory functions which satisfies growth condition

$$g_j(x, u) \leq a|u|^s + b(x), \quad j = \alpha, \beta,$$

for some $a > 0$, $b \in L^1(\Omega)$ and $1 \leq s < \frac{2d}{d-2}$,
and u is the solution of the state equation

$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla u) = f \\ u \in H_0^1(\Omega). \end{cases}$$



Definition (Composite material)

If a sequence of characteristic functions $\chi_\varepsilon \in L^\infty(\Omega; \{0, 1\})$ and conductivities $\mathbf{A}^\varepsilon(x) = \chi_\varepsilon(x)\alpha\mathbf{I} + (1 - \chi_\varepsilon(x))\beta\mathbf{I}$ satisfy

$$\begin{aligned} \chi_\varepsilon &\xrightarrow{*} \theta \\ \mathbf{A}^\varepsilon &\xrightarrow{H} \mathbf{A}, \end{aligned}$$

then it is said that \mathbf{A} is homogenised tensor of two-phase composite material with proportions θ of first material and microstructure defined by the sequence (χ_ε) .

Definition (H-convergence)

A sequence of matrix functions \mathbf{A}^ε is said to H-converge to \mathbf{A} if for every f the sequence of solutions of

$$\begin{cases} -\operatorname{div}(\mathbf{A}^\varepsilon \nabla u_\varepsilon) = f \\ u_\varepsilon \in H_0^1(\Omega) \end{cases}$$

satisfies $u_\varepsilon \rightharpoonup u$ in $H_0^1(\Omega)$, $\mathbf{A}^\varepsilon \nabla u_\varepsilon \rightharpoonup \mathbf{A} \nabla u$ in $L^2(\Omega; \mathbf{R}^d)$, where u is the solution of the homogenised equation

$$\begin{cases} -\operatorname{div}(\mathbf{A} \nabla u) = f \\ u \in H_0^1(\Omega). \end{cases}$$

Example – **simple laminates**: if χ_ε depend only on x_1 , then

$$\mathbf{A} = \operatorname{diag}(\lambda_\theta^-, \lambda_\theta^+, \lambda_\theta^+, \dots, \lambda_\theta^+),$$

where

$$\lambda_\theta^+ = \theta\alpha + (1 - \theta)\beta, \quad \frac{1}{\lambda_\theta^-} = \frac{\theta}{\alpha} + \frac{1 - \theta}{\beta}.$$



Set of all composites:

$$\mathcal{A} := \{(\theta, \mathbf{A}) \in L^\infty(\Omega; [0, 1] \times \mathcal{M}_{\alpha, \beta}) : \mathbf{A} \in \mathcal{K}(\theta) \text{ a.e.}\}$$

G-closure problem: for given θ find all possible homogenised (effective) tensors \mathbf{A}

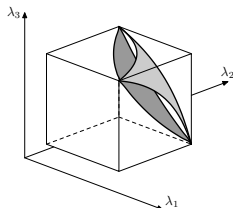
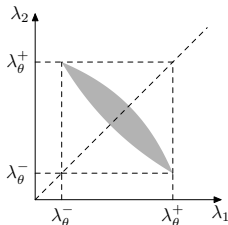
$\mathcal{K}(\theta)$ is given in terms of eigenvalues (Murat & Tartar; Lurie & Cherkaev):

$$\lambda_\theta^- \leq \lambda_j \leq \lambda_\theta^+ \quad j = 1, \dots, d \quad \text{3D:}$$

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

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

2D:





Original problem:

$$\begin{cases} J(\chi) = \int_{\Omega} \chi(\mathbf{x})g_{\alpha}(\mathbf{x}, u) + (1 - \chi(\mathbf{x}))g_{\beta}(\mathbf{x}, u) d\mathbf{x} \longrightarrow \min, \\ \chi \in L^{\infty}(\Omega; \{0, 1\}), \int_{\Omega} \chi d\mathbf{x} = q_{\alpha}. \end{cases}$$

Generalized objective function is

$$J(\theta, \mathbf{A}) = \int_{\Omega} [\theta(\mathbf{x})g_{\alpha}(\mathbf{x}, u(\mathbf{x})) + (1 - \theta(\mathbf{x}))g_{\beta}(\mathbf{x}, u(\mathbf{x}))] d\mathbf{x}$$

where u is the solution of the state equation

$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla u) = f \\ u \in H_0^1(\Omega), \end{cases}$$

and relaxed problem is

$$\begin{cases} J(\theta, \mathbf{A}) \longrightarrow \min, \\ (\theta, \mathbf{A}) \in \mathcal{A}, \int_{\Omega} \theta d\mathbf{x} = q_{\alpha}. \end{cases}$$



Multiple state optimal design problem

State equations

$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla u_i) = f_i \\ u_i \in H_0^1(\Omega) \end{cases} \quad i = 1, \dots, m$$

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

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Relaxed problem:

$$\begin{cases} J(\theta, \mathbf{A}) = \int_{\Omega} (\theta(\mathbf{x})g_{\alpha}(\mathbf{x}, \mathbf{u}) + (1 - \theta(\mathbf{x}))g_{\beta}(\mathbf{x}, \mathbf{u})) d\mathbf{x} \longrightarrow \min \\ (\theta, \mathbf{A}) \in \{(\theta, \mathbf{A}) \in L^{\infty}(\Omega; [0, 1] \times \mathcal{M}_{\alpha, \beta}) : \mathbf{A} \in \mathcal{K}(\theta) \text{ a.e.}\}, \int_{\Omega} \theta d\mathbf{x} = q_{\alpha}. \end{cases}$$



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Optimality condition

- Let (θ^*, \mathbf{A}^*) be optimal point of the relaxed problem and $\varepsilon \mapsto (\theta^\varepsilon, \mathbf{A}^\varepsilon)$ be a smooth path with $(\theta^0, \mathbf{A}^0) = (\theta^*, \mathbf{A}^*)$.
- If $\varepsilon \mapsto J(\theta^\varepsilon, \mathbf{A}^\varepsilon)$ is smooth, then necessary condition of optimality is

$$\delta J(\theta^*, \mathbf{A}^*) := \frac{d}{d\varepsilon} J(\theta^\varepsilon, \mathbf{A}^\varepsilon)|_{\varepsilon=0} \geq 0$$

Let us introduce adjoint states p_1, \dots, p_m as solutions of

$$\begin{cases} -\operatorname{div}(\mathbf{A}\nabla p_i) = \theta \frac{\partial g_\alpha}{\partial u_i}(\cdot, \mathbf{u}) + (1 - \theta) \frac{\partial g_\beta}{\partial u_i}(\cdot, \mathbf{u}) \\ p_i \in H_0^1(\Omega) \end{cases} \quad i = 1, \dots, m.$$

Then

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

for any admissible variation $(\delta\theta, \delta\mathbf{A}) := \left(\frac{d\theta^\varepsilon}{d\varepsilon}, \frac{d\mathbf{A}^\varepsilon}{d\varepsilon} \right) \Big|_{\varepsilon=0}$.



Optimality conditions

How to choose a smooth path?

1. Let us fix θ^* .

a) Then set $\mathcal{K}(\theta^*)$ is convex and we can choose segment

$$\mathbf{A}^\varepsilon = \mathbf{A}^* + \varepsilon(\mathbf{A} - \mathbf{A}^*), \quad \mathbf{A} \in \mathcal{K}(\theta^*)$$

\vdots

[L.Tartar, G. Allaire, M. Vrdoljak]

b) We choose segment in terms of inverse matrices

$$(\mathbf{A}^\varepsilon)^{-1} = (\mathbf{A}^*)^{-1} + \varepsilon(\mathbf{A}^{-1} - (\mathbf{A}^*)^{-1}), \quad \mathbf{A}^{-1} \in \tilde{\mathcal{K}}(\theta^*)$$



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Sets $\mathcal{K}(\theta)$ and $\tilde{\mathcal{K}}(\theta)$

One can show equivalence of the following sets

$\mathcal{K}(\theta)$ - Set of all symmetric matrices \mathbf{A} with eigenvalues $\lambda_1, \dots, \lambda_d$ which satisfies inequalities

$\tilde{\mathcal{K}}(\theta)$ - Set of all symmetric matrices \mathbf{A}^{-1} with eigenvalues ν_1, \dots, ν_d which satisfies inequalities

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

$$\mathbf{A} \in \mathcal{K}(\theta) \Leftrightarrow \mathbf{A}^{-1} \in \tilde{\mathcal{K}}(\theta)$$



Optimality conditions

From necessary condition of optimality

$$- \int_{\Omega} \sum_{i=1}^m \delta \mathbf{A} \nabla u_i^* \cdot \nabla p_i^* d\mathbf{x} \geq 0$$

then follows (for a.e. in Ω)

$$(\mathbf{A}^*)^{-1} : \mathbf{N} = \min_{\mathbf{A} \in \mathcal{K}(\theta^*)} \mathbf{A}^{-1} : \mathbf{N},$$

where $\mathbf{N} = \text{Sym} \sum_{i=1}^m \sigma_i^* \otimes \tau_i^*$, $\sigma_i^* = \mathbf{A}^* \nabla u_i^*$ and $\tau_i^* = \mathbf{A}^* \nabla p_i^*$,
 $i = 1, \dots, m$.



Theorem (von Neumann)

For symmetric matrices \mathbf{A} and \mathbf{M} following inequality is valid

$$A : M \leq \lambda(\mathbf{A}) \cdot \lambda(\mathbf{M}),$$

where $\lambda(\mathbf{A})$ and $\lambda(\mathbf{M})$ are vectors of eigenvalues of \mathbf{A} and \mathbf{M} in nondecreasing order. Equality holds if and only if \mathbf{A} and \mathbf{M} are diagonalizable in same basis.

$$\left\{ \begin{array}{l} \sum_{i=1}^d \nu_i \eta_i \rightarrow \min, \\ \nu_{\theta}^+ \leq \nu_j \leq \nu_{\theta}^-, \quad j = 1, \dots, d \\ \sum_{j=1}^d \frac{1}{\alpha^{-1} - \nu_j} \leq \frac{1}{\alpha^{-1} - \nu_{\theta}^-} + \frac{d-1}{\alpha^{-1} - \nu_{\theta}^+} \\ \sum_{j=1}^d \frac{1}{\nu_j - \beta^{-1}} \leq \frac{1}{\nu_{\theta}^- - \beta^{-1}} + \frac{d-1}{\nu_{\theta}^+ - \beta^{-1}} \end{array} \right.$$

where ν_i are increasing, while η_i decreasing for $i = 1..d$



Optimality conditions

2. Let us now consider variation of θ . We take smooth path $(\theta^\varepsilon, \mathbf{A}^\varepsilon)$ such that a.e. $\mathbf{x} \in \Omega$

$$(\mathbf{A}^\varepsilon)^{-1}(\mathbf{x}) : \mathbf{N}(\mathbf{x}) = \min_{\mathbf{A} \in \mathcal{K}(\theta^\varepsilon)} (\mathbf{A}^{-1}(\mathbf{x}) : \mathbf{N}(\mathbf{x}))$$

Again, from necessary condition of optimality follows (a.e. $\mathbf{x} \in \Omega$)

$$\delta\theta(\mathbf{x}) \left(g_\alpha(\mathbf{x}, \mathbf{u}^*(\mathbf{x})) - g_\beta(\mathbf{x}, \mathbf{u}^*(\mathbf{x})) + l + \frac{\partial g}{\partial \theta}(\theta^*(\mathbf{x}), \mathbf{N}(\mathbf{x})) \right) \geq 0.$$



Theorem

Let (θ^*, \mathbf{A}^*) be minimizer of objective functional $J(\theta, \mathbf{A})$. We introduce symmetric matrix $\mathbf{N} = \text{Sym} \sum_{i=1}^m \sigma_i^* \otimes \tau_i^*$, for $\sigma_i^* = \mathbf{A} \nabla u_i^*$, $\tau_i^* = \mathbf{A} \nabla p_i^*$ and define function $g(\theta, \mathbf{N}) = \min_{\mathbf{A} \in \mathcal{K}(\theta)} (\mathbf{A}^{-1} : \mathbf{N})$. Then

$$(\mathbf{A}^*)^{-1}(\mathbf{x}) : \mathbf{N}(\mathbf{x}) = g(\theta^*(\mathbf{x}), \mathbf{N}(\mathbf{x})), \quad \text{a.e. } x \in \Omega.$$

Moreover, if we define function

$$R(\mathbf{x}) = g_\alpha(\mathbf{x}, \mathbf{u}) - g_\beta(\mathbf{x}, \mathbf{u}) + l + \frac{\partial g}{\partial \theta}(\theta^*(\mathbf{x}), \mathbf{N}^*(\mathbf{x}))$$

the optimal θ^* satisfies (a. e. on Ω)

$$\begin{aligned} \theta^*(\mathbf{x}) &= 0 && \text{if } R(\mathbf{x}) > 0 \\ \theta^*(\mathbf{x}) &= 1 && \text{if } R(\mathbf{x}) < 0 \\ 0 \leq \theta^*(\mathbf{x}) &\leq 1 && \text{if } R(\mathbf{x}) = 0. \end{aligned}$$



Algorithm

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

- 1 Calculate $u_i^k, i = 1, \dots, m$, the solution of

$$\begin{cases} -\operatorname{div}(\mathbf{A}^k \nabla u_i) = f_i \\ u \in H_0^1(\Omega). \end{cases}$$

- 2 Calculate $p_i^k, i = 1, \dots, m$, the solution of

$$\begin{cases} -\operatorname{div}(\mathbf{A}^k \nabla p_i) = \theta^k \frac{\partial g_\alpha}{\partial u_i}(\cdot, \mathbf{u}) + (1 - \theta^k) \frac{\partial g_\beta}{\partial u_i}(\cdot, \mathbf{u}) \\ p_i \in H_0^1(\Omega), \end{cases}$$

$$\sigma_i^k = \mathbf{A}^k \nabla u_i^k, \tau_i^k = \mathbf{A}^k \nabla p_i^k \text{ and } \mathbf{N}^k = \operatorname{Sym} \sum_{i=1}^m (\sigma_i^k \otimes \tau_i^k)$$

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

$$\theta \mapsto g_\alpha(\mathbf{x}, \mathbf{u}^k(\mathbf{x})) - g_\alpha(\mathbf{x}, \mathbf{u}^k(\mathbf{x})) + l + \frac{\partial g}{\partial \theta}(\theta^k, \mathbf{N}^k(\mathbf{x})),$$

if a zero doesn't exist, take 0 (or 1) in case the function is positive (or < 0).

- 4 $(\mathbf{A}^{k+1})^{-1}(\mathbf{x})$ be the minimizer in the definition of $g(\theta^{k+1}(\mathbf{x}), \mathbf{N}^k(\mathbf{x}))$.



Theorem (d=3)

For given $\theta \in [0, 1]$ and matrix \mathbf{N} with eigenvalues $\eta_1 \geq \eta_2 \geq \eta_3$ we have

- A. If $\eta_3 = 0$, then $\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \frac{\beta - \alpha}{(\theta\alpha + (1 - \theta)\beta)^2}(\eta_1 + \eta_2)$.
- B. If $\eta_3 > 0$, then

$$\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \begin{cases} \beta^{-1}(\beta - \alpha)(\alpha + 2\beta) \left(\frac{\sqrt{\eta_1} + \sqrt{\eta_2} + \sqrt{\eta_3}}{2\theta(\alpha - \beta) + \alpha + 2\beta} \right)^2, & \theta < \theta_1^B, \\ \beta^{-1}(\beta^2 - \alpha^2) \left(\frac{\sqrt{\eta_2} + \sqrt{\eta_3}}{\theta(\alpha - \beta) + \alpha + \beta} \right)^2 + \eta_1 \frac{(\beta - \alpha)}{(\theta\alpha + (1 - \theta)\beta)^2}, & \theta_1^B \leq \theta < \theta_2^B, \\ (\alpha^{-1} - \beta^{-1})\eta_3 + \frac{\beta - \alpha}{(\theta\alpha + (1 - \theta)\beta)^2}(\eta_1 + \eta_2), & \theta \geq \theta_2^B, \end{cases}$$

$$\text{where } \theta_1^B = 1 - \frac{\alpha(2\sqrt{\eta_1} - \sqrt{\eta_2} - \sqrt{\eta_3})}{(\beta - \alpha)(\sqrt{\eta_2} + \sqrt{\eta_3} - \sqrt{\eta_1})} \quad \theta_2^B = 1 - \frac{\alpha(\sqrt{\eta_2} - \sqrt{\eta_3})}{(\beta - \alpha)\sqrt{\eta_3}}.$$

- C. Let $\eta_3 < 0$. If η_2 and η_3 are negative as well then

$$\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \begin{cases} -\alpha^{-1}(\beta - \alpha)(2\alpha + \beta) \left(\frac{\sqrt{-\eta_1} + \sqrt{-\eta_2} + \sqrt{-\eta_3}}{2\theta(\alpha - \beta) + 3\beta} \right)^2, & \theta > \theta_1^C, \\ -\alpha^{-1}(\beta^2 - \alpha^2) \left(\frac{\sqrt{-\eta_2} + \sqrt{-\eta_3}}{\theta(\alpha - \beta) + 2\beta} \right)^2 + \eta_1 \frac{\beta - \alpha}{(\theta\alpha + (1 - \theta)\beta)^2}, & \theta_2^C < \theta \leq \theta_1^C, \\ (\alpha^{-1} - \beta^{-1})\eta_3 + \frac{\beta - \alpha}{(\theta\alpha + (1 - \theta)\beta)^2}(\eta_1 + \eta_2), & \theta \leq \theta_2^C. \end{cases}$$

$$\text{where } \theta_1^C = \frac{\beta(\sqrt{-\eta_2} + \sqrt{-\eta_3} - 2\sqrt{-\eta_1})}{(\beta - \alpha)(\sqrt{-\eta_2} + \sqrt{-\eta_3} - \sqrt{-\eta_1})} \quad \text{and } \theta_2^C = \frac{\beta(\sqrt{-\eta_3} - \sqrt{-\eta_2})}{(\beta - \alpha)\sqrt{-\eta_3}}.$$

If $\eta_2 < 0$ and $\eta_1 \geq 0$, then θ_1^C is not defined so we can express $\frac{\partial g}{\partial \theta}(\theta, \mathbf{N})$ by the formulae given above, but omitting its first case and the assumption $\theta \leq \theta_1^C$ in the second case.

If $\eta_2 \geq 0$ then both θ_1^C and θ_2^C are not defined, and $\frac{\partial g}{\partial \theta}(\theta, \mathbf{N})$ is given by the formula given in the third case above, for any $\theta \in [0, 1]$.



Thank you for your attention!