Explicit Hashin-Shtrikman bounds in 3D linearized elasticity and applications

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Teaser

- Problem of explicit bound on 3D composite elastic material made of two isotropic phases
- Open problem for decades
- Everybody knows that it can be solved but no one was willing to undertake the task
- minimization of nonsmooth convex (piecewise quadratic function) in $\mathbf{R}^3$

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Linearized elasticity system

Let $\Omega \subseteq \mathbf{R}^d$ be open and bounded, $\mathbf{A} \in \mathrm{L}^\infty(\Omega; \mathrm{Sym}_\mathrm{d}^4)$ satisfying

$$\mathbf{A}\boldsymbol{\xi} : \boldsymbol{\xi} \geq \alpha|\boldsymbol{\xi}|^2, \quad \mathbf{A}^{-1}\boldsymbol{\xi} : \boldsymbol{\xi} \geq \frac{1}{\beta}|\boldsymbol{\xi}|^2, \qquad \boldsymbol{\xi} \in \mathrm{Sym}_\mathrm{d}$$

and f $\in \mathrm{H}^{-1}(\Omega; \mathbf{R}^\mathrm{d})$. Linearized elasticity system with homogeneous Dirichlet boundary condition:

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

where $e(\mathrm{u}) = \frac{1}{2}(\nabla \mathrm{u} + \nabla \mathrm{u}^\top)$.

Ω - mixture of two isotropic elastic phases with stiffness tensors $\mathbf{A}_1 = 2\mu_1\mathbf{I}_4 + \left(\kappa_1 - \frac{2\mu_1}{d}\right)\mathbf{I}_2 \otimes \mathbf{I}_2$, $\mathbf{A}_2 = 2\mu_2\mathbf{I}_4 + \left(\kappa_2 - \frac{2\mu_2}{d}\right)\mathbf{I}_2 \otimes \mathbf{I}_2$, where $0 < \mu_1 < \mu_2$ and $0 < \kappa_1 < \kappa_2$.

$$\mathbf{A}(\mathbf{x}) = \chi(\mathbf{x})\mathbf{A}_1 + (1 - \chi(\mathbf{x}))\mathbf{A}_2, \quad \chi \in \mathrm{L}^\infty(\Omega; \{0, 1\}).$$

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Composite elastic material

- *fine mixture of materials (on microscale)*
- prevalent in nature, and among engineered materials (sandstone, clouds, bones, wood, concrete, steel and fiberglass)
- they often combine (desired) attributes of the constituent materials

Definition (Composite material)

If a sequence of characteristic functions $\chi_n \in \mathrm{L}^\infty(\Omega; \{0,1\})$ and tensors $\mathbf{A}^n(x) = \chi_n(x)\mathbf{A}_1 + (1 - \chi_n(x))\mathbf{A}_2$ satisfy

$$\begin{aligned} \chi_n &\overset{*}{\rightharpoonup} \theta \\ \mathbf{A}^n &\overset{H}{\rightharpoonup} \mathbf{A}, \end{aligned}$$

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_n).

Definition (H-convergence)

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

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}^n e(\mathsf{u}_n)) = \mathsf{f} \\ \mathsf{u}_n \in \mathrm{H}^1_0(\Omega; \mathbf{R}^d)\,, \end{cases}$$

satisfies $\mathsf{u}_n \rightharpoonup \mathsf{u}$ in $\mathrm{H}^1_0(\Omega; \mathbf{R}^d)$, $\mathbf{A}^n e(\mathsf{u}_n) \rightharpoonup \mathbf{A}e(\mathsf{u})$ in $\mathrm{L}^2(\Omega; \mathrm{Sym}_d)$, where u is the solution of the homogenised equation

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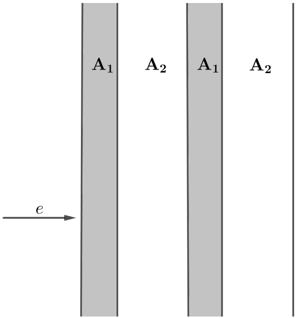
Laminated materials

Simple laminates: if χ_n depend only on x_1, then

$$\theta(\mathbf{A} - \mathbf{A}_2)^{-1} = (\mathbf{A}_1 - \mathbf{A}_2)^{-1} + (1-\theta) f_2(\mathsf{e}_1),$$

where $f_2(\mathsf{e}_1)\boldsymbol{\xi} : \boldsymbol{\xi} = \frac{1}{\mu_2}\left(|\boldsymbol{\xi}\mathsf{e}_1|^2 - (\boldsymbol{\xi}\mathsf{e}_1 \cdot \mathsf{e}_1)^2\right) + \frac{1}{2\mu_2+\lambda_2}(\boldsymbol{\xi}\mathsf{e}_1 \cdot \mathsf{e}_1)^2$, for any $\boldsymbol{\xi} \in \mathrm{Sym_d}$, with $\lambda_2 = \kappa_2 - 2\mu_2/d$.



G–closure and bounds on composites

Set of all composites:

$$\mathcal{A} := \{(\theta, \mathbf{A}) \in \mathrm{L}^\infty(\Omega; [0,1] \times \mathrm{Sym}^4_\mathrm{d}) : \ \mathbf{A}(\mathbf{x}) \in G(\theta(\mathbf{x})) \text{ a.e. } \mathbf{x} \in \Omega\}$$

G–closure problem: for given $\theta \in [0,1]$ find all possible homogenised (effective) tensors $\mathbf{A}$ from $G(\theta)$ – an open problem

Bounds – inequalities correlating various physical and/or microstructural quantities (averaged stress and strain fields, energy, effective stiffness, volume fractions)

Why are they useful?

- quick and simple estimate for the effective tensor
- validation of numerical shemes and experimental results
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Bounds on energy

(Optimal) bounds on $G(\theta)$: for arbitrary $\mathbf{A}^* \in G(\theta)$, $\boldsymbol{\xi} \in \mathrm{Sym_d}$ we have

$$f_-(\theta, \boldsymbol{\xi}) := \min_{\mathbf{A} \in G(\theta)} \mathbf{A}\boldsymbol{\xi} : \boldsymbol{\xi} \leq \mathbf{A}^*\boldsymbol{\xi} : \boldsymbol{\xi} \leq \max_{\mathbf{A} \in G(\theta)} \mathbf{A}\boldsymbol{\xi} : \boldsymbol{\xi} =: f_+(\theta, \boldsymbol{\xi})$$

f_- and f_+ are called lower (upper) Hashin-Shrrikman bounds on *primal* energy

Bounds on *complementary (dual)* energy: for arbitrary $\mathbf{A}^* \in G(\theta)$, $\boldsymbol{\sigma} \in \mathrm{Sym_d}$ we have

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Hashin-Shtrikman bounds

Hashin, Shtrikman (1962, 1963), Allaire, Kohn (1993)

- lower bound on the complementary energy:

$$f_-^c(\theta,\boldsymbol{\sigma}) = \mathbf{A}_2^{-1}\boldsymbol{\sigma}:\boldsymbol{\sigma} + \theta \max_{\boldsymbol{\eta}\in\mathrm{Sym_d}} \left[2\boldsymbol{\sigma}:\boldsymbol{\eta} - (\mathbf{A}_1^{-1} - \mathbf{A}_2^{-1})^{-1}\boldsymbol{\eta}:\boldsymbol{\eta} - (1-\theta)g^c(\boldsymbol{\eta})\right],$$

where $g^c(\boldsymbol{\eta}) = \max_{\mathrm{e}\in S^{d-1}} (f_2^c(\mathrm{e})\boldsymbol{\eta}:\boldsymbol{\eta}) =$

$$= \mathbf{A}_2\boldsymbol{\eta}:\boldsymbol{\eta} - \frac{1}{2\mu_2+\lambda_2}\min\left\{(2\mu_2\eta_1 + \lambda_2\mathrm{tr}(\boldsymbol{\eta}))^2, \ldots, (2\mu_2\eta_d + \lambda_2\mathrm{tr}(\boldsymbol{\eta}))^2\right\}$$

- upper bound on the primal energy:

$$f_+(\theta,\boldsymbol{\xi}) = \mathbf{A}_2\boldsymbol{\xi}:\boldsymbol{\xi} + \theta \min_{\boldsymbol{\eta}\in\mathrm{Sym_d}} \left[2\boldsymbol{\xi}:\boldsymbol{\eta} + (\mathbf{A}_2 - \mathbf{A}_1)^{-1}\boldsymbol{\eta}:\boldsymbol{\eta} - (1-\theta)h(\boldsymbol{\eta})\right],$$

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Explicit Hashin-Shtrikman bounds

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To obtain explicit bound one needs to solve the above nonsmooth convex minimization problem in $\mathbf{R}^d$ with $d+5$ parameters.

d=2:

Gibiansky, Cherkaev (1984) - plate equation, B., Jankov (in preparation)
Allaire, Kohn (1993). Grabovsky (1996), B., Crnjac, Vrdoljak (2021)

d=3: elementary but rather tedious and formidable calculations – a task that no one was willing to undertake
partial results: Allaire (1994), Gibiansky, Cherkaev (1987) - one material being void or rigid

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Hashin-Shtrikman upper bound on the primal energy in 3D

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$$\delta\kappa = \kappa_2-\kappa_1,\ \delta\mu = \mu_2-\mu_1,\ c = \frac{3(1-\theta)}{4\mu_2+3\kappa_2},\ k = \frac{1}{9}\left(\frac{1}{\delta\kappa}-\frac{2}{\delta\mu}\right)\ \mathsf{b} = 2\begin{bmatrix}\xi_1\\ \xi_2\\ \xi_3\end{bmatrix},$$

$$\mathbf{A} = \begin{bmatrix}\frac{1}{2\delta\mu}+k & k & k\\ k & \frac{1}{2\delta\mu}+k & k\\ k & k & \frac{1}{2\delta\mu}+k\end{bmatrix}$$

$$\mathsf{b}\cdot\eta + \max_{1\le i\le 3}\left(\mathbf{A}\eta\cdot\eta - c\eta_i^2\right) \longrightarrow \min_{\eta\in\mathbf{R}^3} \tag{1}$$

$$\begin{cases}\mathsf{b}\cdot\eta + t \longrightarrow \min\limits_{(\eta,t)\in\mathbf{R}^4}\\ \mathbf{A}\eta\cdot\eta - c\eta_i^2 \le t, \quad i=1,2,3\end{cases} \tag{2}$$

Hashin-Shtrikman upper bound on the primal energy in 3D

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Hashin-Shtrikman upper bound on the primal energy in 3D

$$f_+(\theta, \boldsymbol{\xi}) = \mathbf{A}_2\boldsymbol{\xi} : \boldsymbol{\xi} + \theta \min_{\boldsymbol{\eta} \in \mathrm{Sym}_3} \left[2\boldsymbol{\xi} : \boldsymbol{\eta} + (\mathbf{A}_2 - \mathbf{A}_1)^{-1}\boldsymbol{\eta} : \boldsymbol{\eta} - \frac{1-\theta}{2\mu_2 + \lambda_2} \min\left\{\eta_1^2, \eta_2^2, \eta_3^2\right\} \right],$$

$$\delta\kappa = \kappa_2 - \kappa_1,\ \delta\mu = \mu_2 - \mu_1,\ c = \frac{3(1-\theta)}{4\mu_2 + 3\kappa_2},\ k = \frac{1}{9}\left(\frac{1}{\delta\kappa} - \frac{2}{\delta\mu}\right)\ \mathsf{b} = 2\begin{bmatrix}\xi_1\\ \xi_2\\ \xi_3\end{bmatrix},$$

$$\mathbf{A} = \begin{bmatrix} \frac{1}{2\delta\mu} + k & k & k \\ k & \frac{1}{2\delta\mu} + k & k \\ k & k & \frac{1}{2\delta\mu} + k \end{bmatrix}$$

$$\mathsf{b} \cdot \eta + \max_{1 \le i \le 3} \left(\mathbf{A}\eta \cdot \eta - c\eta_i^2\right) \longrightarrow \min_{\eta \in \mathbf{R}^3} \tag{1}$$

$$\begin{cases} \mathsf{b} \cdot \eta + t \longrightarrow \min\limits_{(\eta, t) \in \mathbf{R}^4} \\ \mathbf{A}\eta \cdot \eta - c\eta_i^2 \le t, \quad i = 1, 2, 3 \end{cases} \tag{2}$$

Hashin-Shtrikman upper bound on the primal energy in 3D

Solve it by using Karush-Kuhn-Tucker theorem

High number of parameters makes calculations overwhelming (symbolic computation in Mathematica)

$\delta\mu = \mu_2 - \mu_1$, $\delta\kappa = \kappa_2 - \kappa_1$ and $\gamma_i = 3\kappa_i + 4\mu_i$, $i = 1, 2$, and define the following functions:

$$\begin{aligned}
f(x,y,z) &= (1-\theta)(2\delta\mu(y-z) - 3\delta\kappa(y+2z)) + \gamma_2(z-x) \\
g(x,y,z) &= -3\delta\mu f(x,y,z) - \gamma_2(3\delta\kappa(x+y+z) - 2\delta\mu(-2x+y+z)) \\
l(x,y,z) &= -27(1-\theta)\delta\mu\delta\kappa x + \gamma_2(3\delta\kappa(3x-y+z) + \delta\mu(z-y)) \\
m(x,y,z) &= 9(1-\theta)\delta\kappa x - \gamma_2(2x-y-z).
\end{aligned}$$

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Explicit upper Hashin-Shtrikman bound on the primal energy in 3D

Theorem

In three dimensional, well-ordered case, let $\boldsymbol{\xi}$ *be a symmetric matrix with eigenvalues* ξ_1, ξ_2 *and* ξ_3 *and corresponding orthonormal eigenvectors* e_1, e_2 *and* e_3. *Then, the upper Hashin-Shtrikman bound on primal energy can be expressed explicitly by exactly one of the following five cases. In each case (except the case D) one is free to take any choice* $(i, j, k) \in \{(1, 2, 3), (2, 3, 1), (3, 1, 2)\}$.

A *If*

$$\begin{aligned} f(\xi_i, \xi_j, \xi_k) g(\xi_i, \xi_j, \xi_k) &< 0 \\ f(\xi_i, \xi_k, \xi_j) g(\xi_i, \xi_k, \xi_j) &< 0, \end{aligned} \tag{3}$$

then

$$f_+(\theta, \boldsymbol{\xi}) = (\theta \mathbf{A}_1 + (1-\theta)\mathbf{A}_2)\boldsymbol{\xi} : \boldsymbol{\xi} - (1-\theta)\theta \frac{\big(2\delta\mu(2\xi_i - \xi_j - \xi_k) + 3\delta\kappa(\xi_i + \xi_j + \xi_k)\big)^2}{3\big(\theta\gamma_2 + (1-\theta)\gamma_1\big)}. \tag{4}$$

This bound is achieved by a simple laminate with the lamination direction e_i.

B *If . . .*

E

Equivalence between upper primal bound and lower complementary bound.

For fixed θ, $\frac{1}{2}f_-^c(\theta,\cdot)$ is Legendre-Fenchel transformation of $\frac{1}{2}f_+(\theta,\cdot)$ and vice-versa:

$$\frac{1}{2}f_-^c(\theta,\boldsymbol{\sigma}) = \max_{\boldsymbol{\xi}\in\mathrm{Sym_d}}\left[\boldsymbol{\sigma}:\boldsymbol{\xi} - \frac{1}{2}f_+(\theta,\boldsymbol{\xi})\right]. \tag{5}$$

f_+ is strictly convex in $\boldsymbol{\xi}$ $\Longrightarrow$ f_-^c is smooth in $\boldsymbol{\sigma}$
f_-^cc is strongly convex $\boldsymbol{\sigma}$ $\Longrightarrow$ f_+ is smooth in $\boldsymbol{\xi}$
It holds:

- $\frac{1}{2}f_-^c(\theta,\boldsymbol{\sigma}) = \boldsymbol{\sigma}:\boldsymbol{\xi} - \frac{1}{2}f_+(\theta,\boldsymbol{\xi})\,,$ where $\nabla f_+(\boldsymbol{\xi}) = \boldsymbol{\sigma}$
- ∇f_+ is bijection $\mathrm{Sym_d} \longrightarrow \mathrm{Sym_d}$
- $\mathbf{A}^*$ saturates f_+ if and only if it saturates f_-^c

Thus, we can explicitly calculate the lower complementary bound.

Optimal design problem

For $0 < q < |\Omega|$, f $\in \mathrm{H}^{-1}(\Omega; \mathbf{R}^{\mathrm{d}})$ fixed:

$$
\begin{cases}
J(\chi) := \int_\Omega \mathsf{f}(\mathbf{x}) \cdot \mathsf{u}(\mathbf{x})\, d\mathbf{x} \longrightarrow \min\,, \\
\qquad \chi \in \mathrm{L}^\infty(\Omega; \{0,1\})\,, \ \int_\Omega \chi\, d\mathbf{x} = q\,. \\
\mathbf{A} = \mathbf{A}(\mathbf{x}) = \chi(\mathbf{x})\mathbf{A}_1 + (1-\chi(\mathbf{x}))\mathbf{A}_2 \\
\mathsf{u} \in \mathrm{H}^1_0(\Omega; \mathbf{R}^d) \text{ solves } -\mathrm{div}\,(\mathbf{A} e(\mathsf{u})) = \mathsf{f}
\end{cases}
$$

Solution does not exists!

classical material		composite material - relaxation
$\chi \in \mathrm{L}^\infty(\Omega; \{0,1\})$	$\cdots$	$\theta \in \mathrm{L}^\infty(\Omega; [0,1])$
$\mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}$		$\mathbf{A} \in G(\theta)$ a.e. on Ω

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$\chi \in \mathrm{L}^\infty(\Omega; \{0,1\})$	$\cdots$	$\theta \in \mathrm{L}^\infty(\Omega; [0,1])$
$\mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I}$		$\mathbf{A} \in G(\theta)$ a.e. on Ω
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Optimal design problem

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$$\begin{array}{rcl} \chi \in \mathrm{L}^\infty(\Omega; \{0,1\}) & \cdots & \theta \in \mathrm{L}^\infty(\Omega; [0,1]) \\ \mathbf{A} = \chi\alpha\mathbf{I} + (1-\chi)\beta\mathbf{I} & & \mathbf{A} \in G(\theta) \quad \text{a.e. on } \Omega \\ \text{classical material} & & \text{composite material - relaxation} \end{array}$$

Relaxation by the homogenization method

$$\begin{cases} J(\theta, \mathbf{A}) = \int_\Omega \mathsf{f}(\mathbf{x}) \cdot \mathsf{u}(\mathbf{x})\, d\mathbf{x} + l \int_\Omega \theta(\mathbf{x})\, d\mathbf{x}. \longrightarrow \min\,, \\ (\theta, \mathbf{A}) \in \{(\theta, \mathbf{A}) \in \mathrm{L}^\infty(\Omega; [0,1] \times \mathrm{Sym}_\mathrm{d}^4) : \ \mathbf{A} \in G(\theta) \text{ a.e. on } \Omega\} \\ \mathsf{u} \in \mathrm{H}_0^1(\Omega; \mathbf{R}^d) \text{ solves } -\operatorname{div}(\mathbf{A} e(\mathsf{u})) = \mathsf{f} \end{cases}$$

By the principle of minimal complementary energy we have

$$\min_{(\theta,\mathbf{A})\in\mathcal{A}} J(\theta, \mathbf{A}) = \min_{(\theta,\mathbf{A})\in\mathcal{A}} \min_{\substack{\tau\in\mathrm{L}^2(\Omega;\mathrm{Sym_d}) \\ -\mathrm{div}\tau=\mathsf{f} \text{ in } \Omega}} \int_\Omega \mathbf{A}^{-1}\tau : \tau\, d\mathbf{x} + l \int_\Omega \theta(\mathbf{x})\, d\mathbf{x}.$$

Neccessary conditions of optimality

Theorem

If $(\theta^*, \mathbf{A}^*)$ *is a minimizer of the objective function* J*, and if* $\boldsymbol{\sigma}^*$ *is the unique corresponding minimizer, then* $\boldsymbol{\sigma}^* = \mathbf{A}^* e(\mathrm{u}^*)$*, where* u^* *is the state function for* $(\theta^*, \mathbf{A}^*)$*. Furthermore,* $\mathbf{A}^*$ *satisfies, almost everywhere in* Ω*,*

$$\mathbf{A}^{*-1}\boldsymbol{\sigma}^* : \boldsymbol{\sigma}^* = f_-^c(\theta^*, \boldsymbol{\sigma}^*), \tag{6}$$

while θ^* *is the unique minimizer of the convex minimization problem*

$$\min_{0\leq\theta\leq 1} (f_-^c(\theta, \boldsymbol{\sigma}^*) + l\theta), \quad \text{a.e. on } \Omega. \tag{7}$$

Algorithm

Take some initial θ^0 and $\mathbf{A}^0$. For $k \geq 0$:

1. Calculate u^k, the solution of

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}^k e(\mathsf{u}^k)) = \mathsf{f} \\ \mathsf{u}^k \in \mathrm{H}_0^1(\Omega; \mathbf{R}^d)\,, \end{cases}$$

   and define $\boldsymbol{\sigma}^k := \mathbf{A}^k e(\mathsf{u}^k)$.
2. For $\mathbf{x} \in \Omega$, take $\theta^{k+1}(\mathbf{x})$ as the zero of the function

$$\theta \mapsto \frac{\partial f_-^c}{\partial \theta}(\theta, \boldsymbol{\sigma}^k(\mathbf{x})) + l\,,$$

   and if a zero doesn't exist, take 0 (or 1) if the function is positive (or negative) on $[0, 1]$.
3. Let $(\mathbf{A}^{k+1})(\mathbf{x})$ be the minimizer in the definition of $f_-^c(\theta^{k+1}(\mathbf{x}), \boldsymbol{\sigma}^k(\mathbf{x}))$.

Conclusion

- We have explicitly computed the upper primal bound and the lower complementary Hashin-Shtrikman bound
- it has a number of possible applications in engineering and science of composite materials
- What about lower primal bound and upper complementary bound?

  . . . not the journey that I would take twice

Thank you for your attention!

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