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Towards improved Hashin–Shtrikman bounds on the effective moduli of random composites

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Aug. 27, 2015



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The curse of isotropy

Séba

Aug. 27, 2015



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Towards improved Hashin–Shtrikman bounds on the effective moduli of

The curse of anisotropy

The story of a failure

Aug. 27, 2015



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The principle of minimum potential/complementary energy

Requires kinematically/statically admissible trial fields!

The principle of Hashin & Shtrikman (1962)

The diagram illustrates the Hashin-Shtrikman principle. It features four main components arranged in a diamond shape:

- Local stiffness** (C_0) at the bottom left.
- Stiffness of reference material** (C) at the top left.
- Effective stiffness** (C^{eff}) at the top right.
- Trial field (stress polarization)** ($\mathcal{H}(\hat{\tau})$) at the bottom right.

Curved arrows indicate the relationships between these components:

- A curved arrow from C_0 to C is labeled with a red " \leq " symbol above it and a blue " \geq " symbol below it.
- A curved arrow from C to C^{eff} is labeled with a red " \leq " symbol above it and a blue " \geq " symbol below it.
- A curved arrow from C^{eff} to $\mathcal{H}(\hat{\tau})$ is labeled with a red " \leq " symbol above it and a blue " \geq " symbol below it.
- A curved arrow from $\mathcal{H}(\hat{\tau})$ back to C_0 is labeled with a red " \leq " symbol above it and a blue " \geq " symbol below it.

To the right of the diagram, the text "No requirements on the trial field!" is written in red.

Below the diagram, the text "Functional of H&S (TBD later)" is written in red.

Hashin & Shtrikman (1962), *J. Mech. Phys. Sol.* **10**(4)

Willis (1977), *J. Mech. Phys. Sol.* **25**(3)

Phase-wise constant trial fields: the most simple trial field

$$\hat{\boldsymbol{\tau}}(\boldsymbol{x}) = \sum_{\alpha=1}^N \chi_\alpha(\boldsymbol{x}) \hat{\boldsymbol{\tau}}_\alpha$$

Indicator function of phase α Constant (to be optimized)

Local descriptors of the microstructure

The χ_α at the observation point.

Macroscopic descriptors (Hashin and Shtrikman, 1962)

Volume fractions only (isotropic materials)!

Phase-wise constant trial fields

- do not depend on neighborhood
- no (relative) length-scale in the resulting bounds

Additional local descriptors

- should remain simple (for evaluation of $\mathcal{H}(\hat{\tau})$)
- aggregate microstructural info **at** and **around** observation point

The most simple such local descriptor

- local volume fraction
- arguably physically meaningful (Widjajakusuma et al., 1999)

Widjajakusuma et al. (1999), *Comput. Mater. Sci.* **16**(1-4)

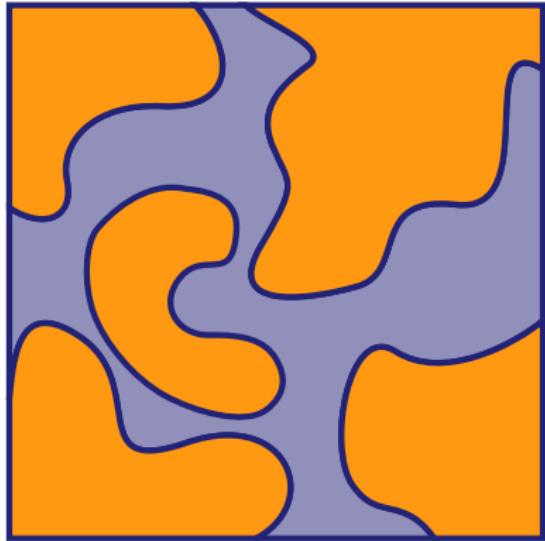
Spherical windows

$$\tilde{f}_\alpha(x, a) = \frac{1}{W} \int_{\|r\| \leq a} \chi_\alpha(x + r) dV_r$$

Radius of spherical window

Indicator function of phase α

Volume of spherical window



The case of two-phase materials

$$\tilde{f}(x, a) = \tilde{f}_1(x, a) = 1 - \tilde{f}_2(x, a)$$

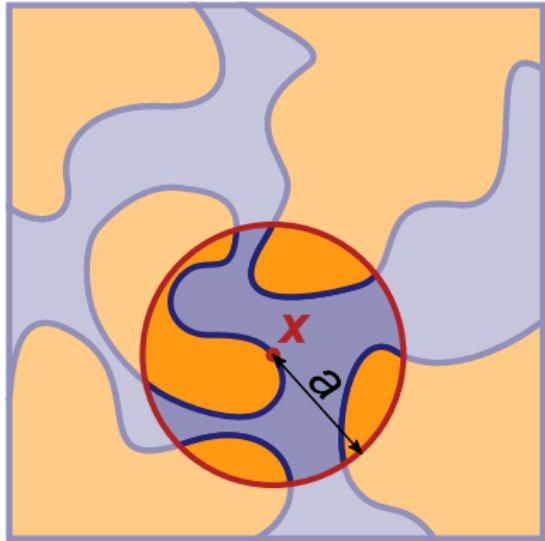
Spherical windows

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Radius of spherical window

Indicator function of phase α

Volume of spherical window



The case of two-phase materials

$$\tilde{f}(x, a) = \tilde{f}_1(x, a) = 1 - \tilde{f}_2(x, a)$$

Step 1 – Defining enriched trial fields

Step 2 – Evaluating the H&S functional → The curse of isotropy!

Step 3 – Optimizing the resulting bound

Step 1 – Defining enriched trial fields

Original trial field

$$\hat{\boldsymbol{\tau}}(\boldsymbol{x}) = \sum_{\alpha=1}^2 \chi_\alpha(\boldsymbol{x}) \hat{\boldsymbol{\tau}}_\alpha$$

Enriched trial field

$$\hat{\boldsymbol{\tau}}(\boldsymbol{x}) = \sum_{\alpha=1}^2 \sum_{h=1}^p \chi_\alpha(\boldsymbol{x}) \tilde{f}(\boldsymbol{x}, \boldsymbol{a})^h \hat{\boldsymbol{\tau}}_{\alpha h}$$

Constant (to be optimized)

The functional of Hashin & Shtrikman

$$\mathcal{H}(\hat{\boldsymbol{\tau}}) = \frac{1}{2} \boldsymbol{E} : \boldsymbol{C}_0 : \boldsymbol{E} + \boxed{\boldsymbol{E} : \bar{\boldsymbol{\tau}}} - \frac{1}{2} \boxed{\hat{\boldsymbol{\tau}} : (\boldsymbol{C} - \boldsymbol{C}_0)^{-1} : \hat{\boldsymbol{\tau}}} - \frac{1}{2} \boxed{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]}$$

The functional of Hashin & Shtrikman

$$\mathcal{H}(\hat{\boldsymbol{\tau}}) = \frac{1}{2} \mathbf{E} : \mathbf{C}_0 : \mathbf{E} + \boxed{\mathbf{E} : \hat{\boldsymbol{\tau}}} - \frac{1}{2} \boxed{\hat{\boldsymbol{\tau}} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \hat{\boldsymbol{\tau}}} - \frac{1}{2} \boxed{\hat{\boldsymbol{\tau}} : \Gamma_0[\hat{\boldsymbol{\tau}}]}$$

The equation shows the Hashin-Shtrikman functional $\mathcal{H}(\hat{\boldsymbol{\tau}})$. It consists of four terms. The first term is the energy of the elastic tensor \mathbf{E} relative to the reference tensor \mathbf{C}_0 . The second term is the energy of the stress tensor $\hat{\boldsymbol{\tau}}$ relative to the identity tensor. The third term is the energy of the stress tensor $\hat{\boldsymbol{\tau}}$ relative to the compliance tensor $(\mathbf{C} - \mathbf{C}_0)^{-1}$. The fourth term is the energy of the stress tensor $\hat{\boldsymbol{\tau}}$ relative to the compliance tensor $\Gamma_0[\hat{\boldsymbol{\tau}}]$. Brackets group the terms into pairs: the first pair is the energy of the stress tensor relative to the identity tensor and the second pair is the energy of the stress tensor relative to the compliance tensor. Arrows from the top equation point to these brackets.

One-point descriptors of the microstructure

$$Y_{\alpha h} = \langle \chi_\alpha(x) \tilde{f}(x, a)^h \rangle$$

The functional of Hashin & Shtrikman

$$\mathcal{H}(\hat{\boldsymbol{\tau}}) = \frac{1}{2} \mathbf{E} : \mathbf{C}_0 : \mathbf{E} + \boxed{\mathbf{E} : \hat{\boldsymbol{\tau}}} - \frac{1}{2} \boxed{\hat{\boldsymbol{\tau}} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \hat{\boldsymbol{\tau}}} - \frac{1}{2} \boxed{\hat{\boldsymbol{\tau}} : \Gamma_0[\hat{\boldsymbol{\tau}}]}$$

The equation shows the Hashin-Shtrikman functional $\mathcal{H}(\hat{\boldsymbol{\tau}})$. It consists of four terms: 1) A constant term $\frac{1}{2} \mathbf{E} : \mathbf{C}_0 : \mathbf{E}$. 2) A term involving the compliance tensor \mathbf{E} and the stress tensor $\hat{\boldsymbol{\tau}}$, enclosed in a blue box. 3) A term involving the inverse compliance tensor $(\mathbf{C} - \mathbf{C}_0)^{-1}$ and the stress tensor $\hat{\boldsymbol{\tau}}$, enclosed in a blue box. 4) A term involving the compliance tensor Γ_0 and the stress tensor $\hat{\boldsymbol{\tau}}$, enclosed in a red box. Arrows from the first two terms point to a bracketed sum above them, and arrows from the last two terms point to another bracketed sum above them.

One-point descriptors of the microstructure

???

$$Y_{\alpha h} = \langle \chi_\alpha(x) \tilde{f}(x, a)^h \rangle$$

The Green operator for strains as a “convolution” operator

$$\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \frac{1}{V} \int_{x,y \in \Omega} \hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x, y) : \hat{\boldsymbol{\tau}}(y) dV_x dV_y$$

The Green operator for strains as a “convolution” operator

$$\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \frac{1}{V} \int_{x,y \in \Omega} \hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x, y) : \hat{\boldsymbol{\tau}}(y) dV_x dV_y$$

If Ω is indeed a RVE, then $\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \langle \overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} \rangle$

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The Green operator for strains as a “convolution” operator

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$$\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \frac{1}{V} \int_{x,y \in \Omega} \langle \hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x, y) : \hat{\boldsymbol{\tau}}(y) \rangle dV_x dV_y$$

$$\langle \hat{\boldsymbol{\tau}}(x) : \boldsymbol{\Gamma}_0(x, y) : \hat{\boldsymbol{\tau}}(y) \rangle = \sum_{\alpha, \beta, h, k} Z_{\alpha h, \beta k}(x - y) \hat{\boldsymbol{\tau}}_{\alpha h} : \boldsymbol{\Gamma}_0(x, y) : \hat{\boldsymbol{\tau}}_{\beta k}$$

Two-point descriptors of the microstructure

$$Z_{\alpha h, \beta k}(\mathbf{r}) = \langle \chi_\alpha(\mathbf{x}) \tilde{f}(\mathbf{x}, \mathbf{a})^h \chi_\beta(\mathbf{x} + \mathbf{r}) \tilde{f}(\mathbf{x} + \mathbf{r}, \mathbf{a})^k \rangle$$

For isotropic microstructures

$$Z_{\alpha h, \beta k}(\mathbf{r}) = Z_{\alpha h, \beta k}(\|\mathbf{r}\|)$$

Two-point descriptors vanish!

$$\frac{1}{V} \int Z_{\alpha h, \beta k}(\mathbf{x} - \mathbf{y}) \Gamma_0(\mathbf{x}, \mathbf{y}) dV_x dV_y = (Y_{\alpha, h+k} \delta_{\alpha\beta} - Y_{\alpha h} Y_{\beta k}) P_0$$

Hill tensor of spheres

Step 2 – Evaluating the H&S functional

Putting it all together

$$\mathcal{H}(\hat{\boldsymbol{\tau}}) = \frac{1}{2} \mathbf{E} : \mathbf{C}_0 : \mathbf{E} + \boxed{\mathbf{E} : \bar{\hat{\boldsymbol{\tau}}}} - \frac{1}{2} \boxed{\hat{\boldsymbol{\tau}} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \hat{\boldsymbol{\tau}}} - \frac{1}{2} \boxed{\hat{\boldsymbol{\tau}} : \Gamma_0[\hat{\boldsymbol{\tau}}]}$$

$\sum_{\alpha,h,k} Y_{\alpha,h+k} \hat{\boldsymbol{\tau}}_{\alpha h} : (\mathbf{C}_\alpha - \mathbf{C}_0)^{-1} : \hat{\boldsymbol{\tau}}_{\alpha k}$

$\sum_{\alpha,h} Y_{\alpha h} \mathbf{E} : \hat{\boldsymbol{\tau}}_{\alpha h}$

$\sum_{\alpha,h,\beta,k} (Y_{\alpha,h+k} \delta_{\alpha\beta} - Y_{\alpha h} Y_{\beta k}) \hat{\boldsymbol{\tau}}_{\alpha h} : \mathbf{P}_0 : \hat{\boldsymbol{\tau}}_{\beta k}$

Step 3 – Optimizing the bound w.r.t $\hat{\tau}_{\alpha h}$

Stationarity conditions

$$\sum_k Y_{\alpha,h+k} \left((\mathbf{C}_\alpha - \mathbf{C}_0)^{-1} + \mathbf{P}_0 \right) : \hat{\boldsymbol{\tau}}_{\alpha k} = Y_{\alpha h} \left(\mathbf{E} + \sum_{\beta,k} Y_{\beta k} \mathbf{P}_0 : \hat{\boldsymbol{\tau}}_{\beta k} \right)$$

Solving the linear system

$$\hat{\boldsymbol{\tau}}_{\alpha k} = \mathbf{0} \text{ for } k \neq 0!$$

Remember

$$\hat{\boldsymbol{\tau}}(\mathbf{x}) = \sum_{\alpha,k} \chi_\alpha(\mathbf{x}) \tilde{f}(\mathbf{x}, \mathbf{a})^k \hat{\boldsymbol{\tau}}_{\alpha k}$$

Standard bounds of H&S are retrieved :-)

All these developments for nothing?

- Enrichment led to no improvement!
- Extends to a wider class of trial fields!

However...

- Approach might apply to other situations.
- Was well worth trying (if only to spare the time of others!).

Perspectives

- Analysis suggests enrichments with better prospects (maybe).
- Isotropy is the root of our misfortunes: anisotropic descriptors?

$$\langle \chi_\alpha(x) \Phi_h(x) \chi_\beta(x + rn) \Phi_k(x + rn) \rangle = \text{func.}(r, \textcolor{red}{n})$$

Thank you for your attention!

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<http://sbrisard.github.io/>

Paper number 68474 (also on HAL)

Field equations

$$\nabla \cdot \boldsymbol{\sigma}(x) = \mathbf{0}$$

$$\boldsymbol{\sigma}(x) = \mathbf{C}(\textcolor{red}{x}) : \boldsymbol{\epsilon}(x) \iff \nabla \cdot (\mathbf{C} : \nabla^s \mathbf{u}) = \mathbf{0}$$

$$\boldsymbol{\epsilon}(x) = \nabla^s \mathbf{u}(x)$$

Boundary conditions

$$\mathbf{u}(x) = \mathbf{E} \cdot \mathbf{x} \iff \mathbf{u} \text{ k.a. with } \mathbf{E}$$

k.a. = *kinematically admissible*.

Effective properties

$$\mathbf{C}^{\text{eff}} = \overline{\boldsymbol{\sigma}} = \overline{\mathbf{C} : \boldsymbol{\epsilon}}$$

Introducing an arbitrary, homogeneous reference material C_0 .

The Green operator for strains

$$\left. \begin{aligned} & \nabla \cdot (C_0 : \nabla^s u + \tau) \\ & u \text{ k.a. with } 0 \end{aligned} \right\} \iff \epsilon = -\Gamma_0[\tau]$$

The Lippmann–Schwinger equation

$$\left. \begin{aligned} & \nabla \cdot (C : \nabla^s u) \\ & u \text{ k.a. with } E \end{aligned} \right\} \iff \epsilon = E - \Gamma_0[(C - C_0) : \epsilon]$$

$$\iff \begin{cases} (C - C_0)^{-1} : \tau + \Gamma_0[\tau] = E \\ \tau = (C - C_0) : \epsilon \end{cases}$$

Basic properties

$$\langle \tilde{f}_\alpha(x, a) \rangle = f_\alpha$$

$$\langle \tilde{f}_\alpha^2(x, 0) \rangle = f_\alpha$$

$$\langle \tilde{f}_\alpha^2(x, +\infty) \rangle = 0$$

Example: hard spheres

- d : diameter,
- $f = 0.4$,
- 2048 spheres,
- 10000 realizations.

