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

Sébastien Brisard

Aug. 27, 2015



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

The curse of isotropy

Séba

Aug. 27, 2015



Towards improved Hashin–Shtrikman bounds on the effective modulus of random polycrystals

The cure
The story of a failure
isotropy

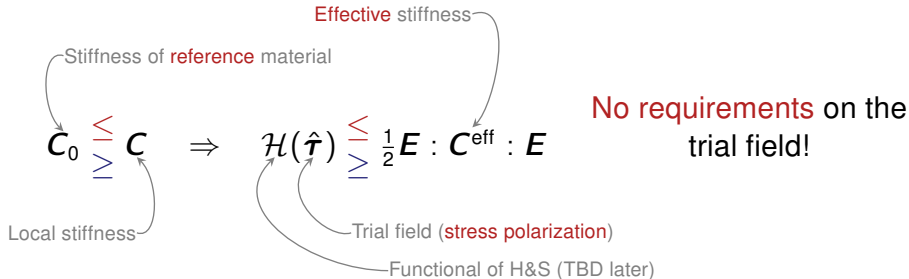
Aug. 27, 2015



The principle of minimum potential/complementary energy

Requires **kinematically/statically admissible** trial fields!

The principle of Hashin & Shtrikman (1962)



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

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

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)**

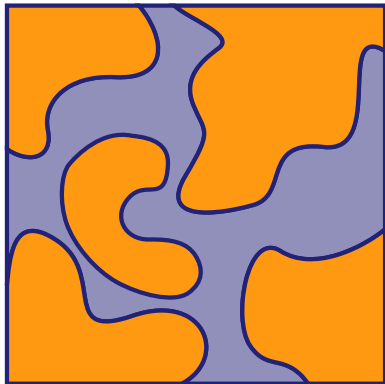
Spherical windows

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

Radius of spherical window

Indicator function of phase α

Volume of spherical window



The case of two-phase materials

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

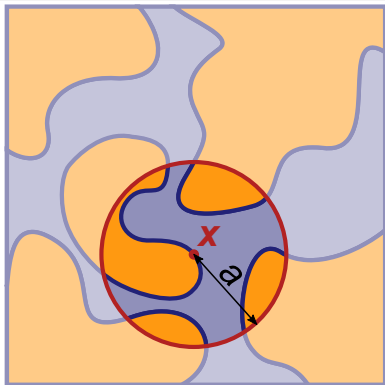
Spherical windows

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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

Original trial field

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

Enriched trial field

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

Constant (to be optimized)



The functional of Hashin & Shtrikman

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

The functional of Hashin & Shtrikman

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

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

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

One-point descriptors of the microstructure

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

The functional of Hashin & Shtrikman

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

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

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One-point descriptors of the microstructure

???

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

The Green operator for strains as a “convolution” operator

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

The Green operator for strains as a “convolution” operator

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

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

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The Green operator for strains as a “convolution” operator

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

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

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!

Hill tensor of spheres

$$\frac{1}{V} \int Z_{\alpha h, \beta k}(\mathbf{x} - \mathbf{y}) \Gamma_0(\mathbf{x}, \mathbf{y}) dV_x dV_y = (Y_{\alpha, h+k} \delta_{\alpha\beta} - Y_{\alpha h} Y_{\beta k}) \mathbf{P}_0$$

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

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

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

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

Stationarity conditions

$$\sum_k Y_{\alpha, h+k} \left((C_\alpha - C_0)^{-1} + P_0 \right) : \hat{\tau}_{\alpha k} = Y_{\alpha h} \left(E + \sum_{\beta, k} Y_{\beta k} P_0 : \hat{\tau}_{\beta k} \right)$$

Solving the linear system

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

Remember

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

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?

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

Thank you for your attention!

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Paper number 68474 (also on HAL)

Field equations

$$\begin{aligned}\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) &= \mathbf{0} \\ \boldsymbol{\sigma}(\mathbf{x}) &= \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x}) \iff \nabla \cdot (\mathbf{C} : \nabla^s \mathbf{u}) = \mathbf{0} \\ \boldsymbol{\varepsilon}(\mathbf{x}) &= \nabla^s \mathbf{u}(\mathbf{x})\end{aligned}$$

Boundary conditions

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

k.a. = *kinematically admissible*.

Effective properties

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

Introducing an arbitrary, homogeneous reference material \mathbf{C}_0 .

The Green operator for strains

$$\left. \begin{array}{l} \nabla \cdot (\mathbf{C}_0 : \nabla^s \mathbf{u} + \boldsymbol{\tau}) \\ \mathbf{u} \text{ k.a. with } \mathbf{0} \end{array} \right\} \iff \boldsymbol{\varepsilon} = -\Gamma_0[\boldsymbol{\tau}]$$

The Lippmann–Schwinger equation

$$\left. \begin{array}{l} \nabla \cdot (\mathbf{C} : \nabla^s \mathbf{u}) \\ \mathbf{u} \text{ k.a. with } \mathbf{E} \end{array} \right\} \iff \boldsymbol{\varepsilon} = \mathbf{E} - \Gamma_0[(\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon}]$$

$$\iff \begin{cases} (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \Gamma_0[\boldsymbol{\tau}] = \mathbf{E} \\ \boldsymbol{\tau} = (\mathbf{C} - \mathbf{C}_0) : \boldsymbol{\varepsilon} \end{cases}$$

Basic properties

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

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

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

Example: hard spheres

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

