



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

Sébastien Brisard

► To cite this version:

Sébastien Brisard. Towards improved Hashin–Shtrikman bounds on the effective moduli of random composites. 22ème Congrès Français de Mécanique, Aug 2015, Lyon, France. hal-01187829

HAL Id: hal-01187829

<https://enpc.hal.science/hal-01187829>

Submitted on 27 Aug 2015

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution - NonCommercial 4.0 International License

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

Sébastien Brisard

Aug. 27, 2015



UNIVERSITÉ —
PARIS-EST



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

The curse of isotropy
Sébastien
Aug. 27, 2015



UNIVERSITÉ —
PARIS-EST



Towards improved Hashin–Shtrikman bounds on the effective moduli of

The curse of anisotropy

The story of a failure

Aug. 27, 2015



UNIVERSITÉ —
PARIS-EST



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 circle:

- Local stiffness** (C_0)
- Stiffness of reference material** (C)
- Effective stiffness** (C^{eff})
- Trial field (stress polarization)** ($\mathcal{H}(\hat{\tau})$)

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

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)

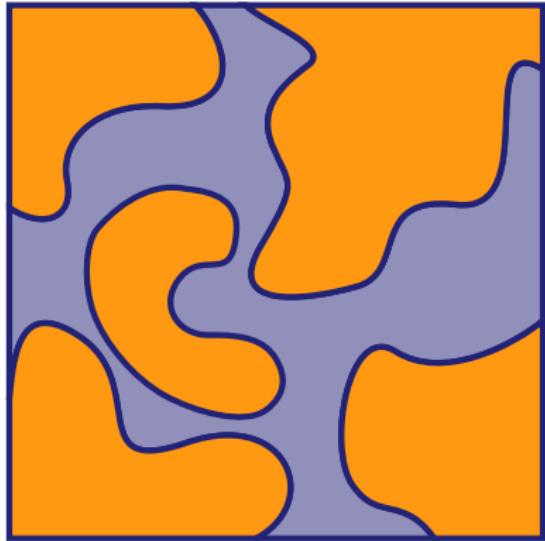
Spherical windows

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

Radius of spherical window

Indicator function of phase α

Volume of spherical window



The case of two-phase materials

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

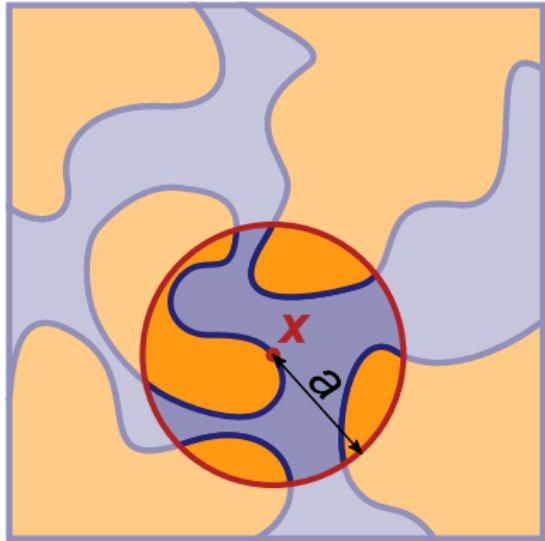
Spherical windows

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

Radius of spherical window

Indicator function of phase α

Volume of spherical window



The case of two-phase materials

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

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 are used to group terms: curly braces group the second and third terms, and rectangular boxes group the second, third, and fourth terms.

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. The first term is the energy of the reference configuration. The second term is the energy of the current configuration. The third term is the energy due to the constraint that the current configuration is a deformation of the reference configuration. The fourth term is the energy due to the constraint that the current configuration is a solution to the eigenvalue problem of the linearized elastic operator Γ_0 .

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 $\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \langle \overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} \rangle$

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

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 $\overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} = \langle \overline{\hat{\boldsymbol{\tau}} : \boldsymbol{\Gamma}_0[\hat{\boldsymbol{\tau}}]} \rangle$

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

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

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

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

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

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

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

The diagram illustrates the mapping from the components of the H&S functional to the terms in the equation. Arrows point from the first term in the H(S) functional ($\mathbf{E} : \bar{\hat{\boldsymbol{\tau}}}$) to the second term in the sum ($Y_{\alpha h} \hat{\boldsymbol{\tau}}_{\alpha h}$), from the second term in the H(S) functional ($\hat{\boldsymbol{\tau}} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \hat{\boldsymbol{\tau}}$) to the third term in the sum ($Y_{\alpha,h+k} \hat{\boldsymbol{\tau}}_{\alpha h} : (\mathbf{C}_\alpha - \mathbf{C}_0)^{-1} : \hat{\boldsymbol{\tau}}_{\alpha k}$), and from the third term in the H(S) functional ($\hat{\boldsymbol{\tau}} : \Gamma_0[\hat{\boldsymbol{\tau}}]$) to the fourth term in the sum ($(Y_{\alpha,h+k} \delta_{\alpha\beta} - Y_{\alpha h} Y_{\beta k}) \hat{\boldsymbol{\tau}}_{\alpha h} : \mathbf{P}_0 : \hat{\boldsymbol{\tau}}_{\beta k}$).

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!

sebastien.brisard@ifsttar.fr

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

Paper number 68474 (also on HAL)

Field equations

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

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

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

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.

