



Beyond the classical Hashin–Shtrikman bounds: the Hashin–Shtrikman principle revisited

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Beyond the classical Hashin–Shtrikman bounds

The Hashin–Shtrikman principle revisited

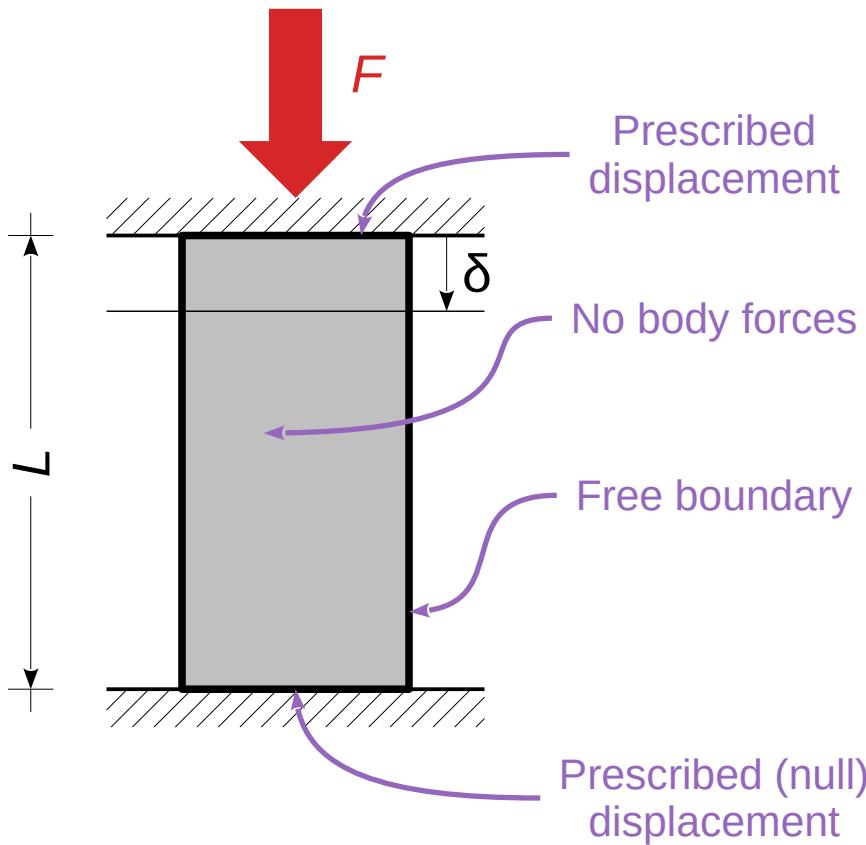
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Experimental homogenization

Effective moduli measured through simple uniaxial test



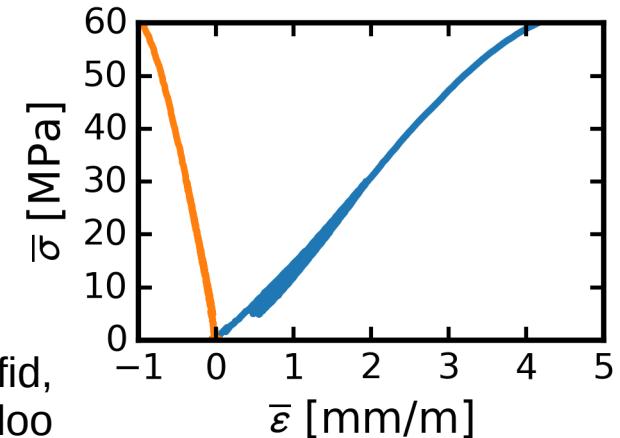
Macroscopic strain & stress

$$\bar{\epsilon} = \frac{\delta}{L} \quad \bar{\sigma} = \frac{F}{S}$$

Effective Young modulus

$$E = \frac{\bar{\sigma}}{\bar{\epsilon}}$$

Courtesy S. Bahafid,
S. Ghabezloo

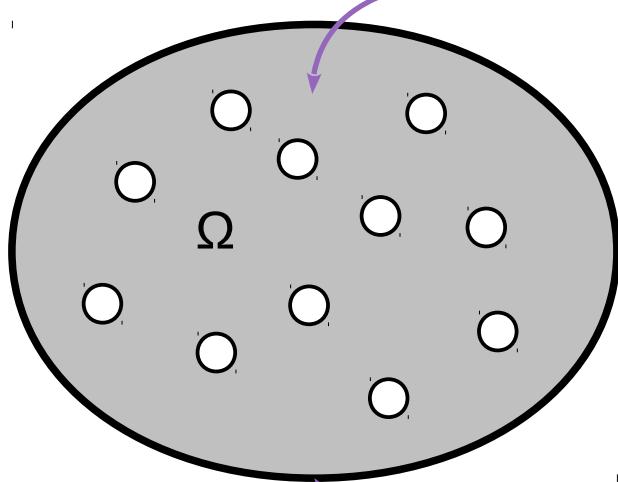


Loading conditions are such that

$$\bar{\epsilon} = \langle \epsilon \rangle \quad \bar{\sigma} = \langle \sigma \rangle \quad \bar{\sigma} \bar{\epsilon} = \langle \sigma \epsilon \rangle$$

Numerical homogenization

The corrector problem



No body forces

Field equations (in Ω)

$$\operatorname{div} \boldsymbol{\sigma} = 0$$

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\epsilon}$$

$$\boldsymbol{\epsilon} = \text{sym grad } \mathbf{u}$$

Imposed
displacement

Boundary conditions (on $\partial\Omega$)

$$\mathbf{u}(\mathbf{x}) = \bar{\boldsymbol{\epsilon}} \cdot \mathbf{x}$$

BCs ensure that

$$\langle \boldsymbol{\epsilon} \rangle = \bar{\boldsymbol{\epsilon}}$$

Effective moduli

$$\langle \boldsymbol{\sigma} : \boldsymbol{\epsilon} \rangle = \langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\epsilon} \rangle$$

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

The homogenization toolkit

Pros

- ✓ Simple
- ✓ Versatile

Cons

- ✗ No correlations
- ✗ Restricted to ellipsoids!

Pros

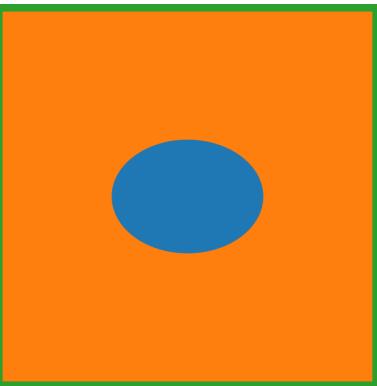
- ✓ Captures fine details of microstructure

Cons

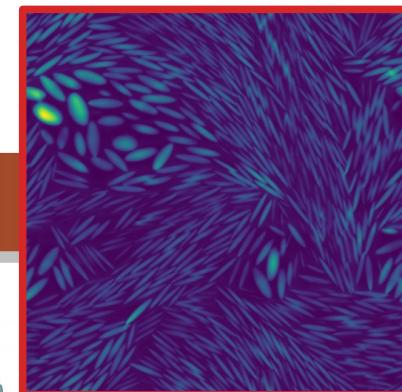
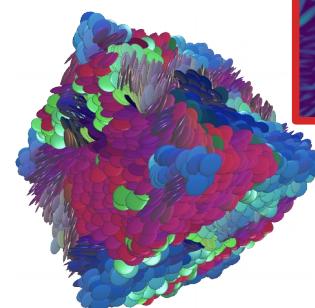
- ✗ Time consuming
- ✗ Difficult to analyze



Complexity



Mean-field
methods



Full-field
methods

Outline of this talk

- ▶ Variational methods for homogenization
- ▶ Polarization techniques for homogenization:
the Hashin–Shtrikman principle
- ▶ Realization-by-realization applications of the HS principle
(FFT-based methods, EIM)
- ▶ Statistical applications of the HS principle: classical and improved HS bounds



Varational methods for homogenization

Variational methods

The true solution of the corrector problem

- ▶ Minimizes some energy
- ▶ Trial fields must be **admissible**

Construction of an approximate solution?

- ▶ Construct a **subspace** of admissible trial fields
- ▶ Minimize energy over this subspace

How to select “good” trial fields?

Minimum of potential energy

Potential energy

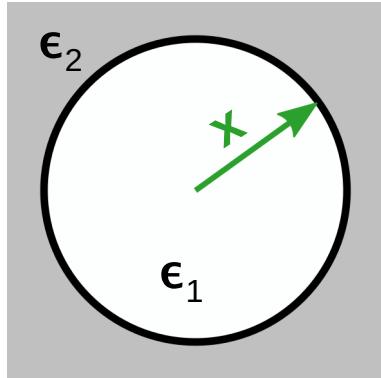
$$\Pi(\boldsymbol{\epsilon}) = \frac{1}{2} \langle \boldsymbol{\epsilon} : \mathbf{C} : \boldsymbol{\epsilon} \rangle \geq \frac{1}{2} \bar{\boldsymbol{\epsilon}} : \mathbf{C}^{\text{eff}} : \bar{\boldsymbol{\epsilon}}$$

Admissible trial strain

$$\text{In } \Omega: \boldsymbol{\epsilon} = \mathbf{sym} \mathbf{grad} \mathbf{u}$$

$$\text{On } \partial\Omega: \mathbf{u} = \bar{\boldsymbol{\epsilon}} \cdot \mathbf{x}$$

Simple admissible trial strain?



- ▶ Try phase-wise constant strains
 $\mathbf{u}(\mathbf{x}) = \boldsymbol{\epsilon}_\alpha \cdot \mathbf{x}$ for \mathbf{x} in phase α
- ▶ Displacement is continuous
 $\boldsymbol{\epsilon}_1 \cdot \mathbf{x} = \boldsymbol{\epsilon}_2 \cdot \mathbf{x}$ on the interface

Constant strain field!!!

$$\mathbf{C}^{\text{eff}} \leq \langle \mathbf{C} \rangle \quad (\text{Voigt})$$

Minimum of complementary energy

Complementary energy

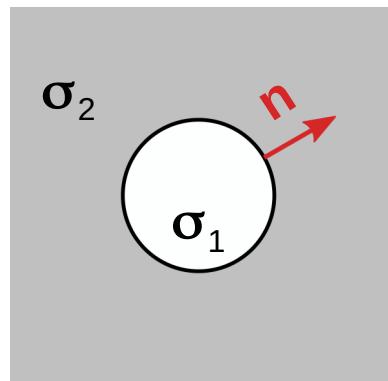
$$\Pi^*(\sigma) = \frac{1}{2} \langle \sigma : \mathbf{S} : \sigma \rangle \geq \frac{1}{2} \bar{\sigma} : \mathbf{S}^{\text{eff}} : \bar{\sigma}$$

Admissible trial stress

$$\text{In } \Omega: \operatorname{div} \sigma = 0$$

$$\text{On } \partial\Omega: \sigma \cdot \mathbf{n} = \bar{\sigma} \cdot \mathbf{n}$$

Simple admissible trial stress?



► Try phase-wise constant stresses

$$\sigma(\mathbf{x}) = \sigma_\alpha \text{ for } \mathbf{x} \text{ in phase } \alpha$$

► Traction is continuous

$$\sigma_1 \cdot \mathbf{n} = \sigma_2 \cdot \mathbf{n} \text{ on the interface}$$

Constant trial stress!!!

$$\mathbf{C}^{\text{eff}} \geq \langle \mathbf{S}^{-1} \rangle^{-1} \quad (\text{Reuss})$$

Polarization techniques for homogenization

The Green operator for strains

The initial, corrector problem

$$\operatorname{div} \boldsymbol{\sigma} = 0$$

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\epsilon}$$

$$\boldsymbol{\epsilon} = \operatorname{sym} \operatorname{grad} \mathbf{u}$$

$$\boldsymbol{\epsilon} \in \mathbf{KA}(\bar{\boldsymbol{\epsilon}})$$

A new, auxiliary problem

$$\operatorname{div} \boldsymbol{\sigma} = 0$$

$$\boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\epsilon} + \boldsymbol{\tau}$$

$$\boldsymbol{\epsilon} = \operatorname{sym} \operatorname{grad} \mathbf{u}$$

$$\boldsymbol{\epsilon} \in \mathbf{KA}(\bar{\boldsymbol{\epsilon}})$$

- ▶ Reference material \mathbf{C}_0 is homogeneous
- ▶ Stress-polarization $\boldsymbol{\tau}$ is heterogeneous
- ▶ Solution depends linearly on $\boldsymbol{\tau}, \bar{\boldsymbol{\epsilon}}$

Korringa, J. Math. Phys. 14(4), 1973

Zeller & Dederichs, Physica Status Solidi (B) 55(2), 1973

$$\boldsymbol{\epsilon} = \bar{\boldsymbol{\epsilon}} - \boldsymbol{\Gamma}_0[\boldsymbol{\tau}]$$

The Lippmann–Schwinger equation

The initial problem

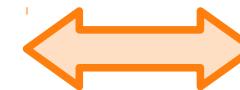
Introducing the
stress-polarization

By definition of the
Green operator

$$\begin{aligned} \operatorname{div} \sigma &= 0 \\ \sigma &= \mathbf{C} : \epsilon \\ \epsilon &= \operatorname{sym} \operatorname{grad} \mathbf{u} \\ \epsilon &\in \mathbf{KA}(\bar{\epsilon}) \end{aligned}$$



$$\begin{aligned} \operatorname{div} \sigma &= 0 \\ \sigma &= \mathbf{C}_0 : \epsilon + \tau \\ \epsilon &= \operatorname{sym} \operatorname{grad} \mathbf{u} \\ \epsilon &\in \mathbf{KA}(\bar{\epsilon}) \\ \tau &= (\mathbf{C} - \mathbf{C}_0) : \epsilon \end{aligned}$$



$$\epsilon = \bar{\epsilon} - \Gamma_0[\tau]$$



$$\tau = (\mathbf{C} - \mathbf{C}_0) : \epsilon$$

$$(\mathbf{C} - \mathbf{C}_0)^{-1} : \tau + \Gamma_0[\tau] = \bar{\epsilon}$$

Korringa, J. Math. Phys. 14(4), 1973

Zeller & Dederichs, Physica Status Solidi (B) 55(2), 1973

The Hashin–Shtrikman principle (1/3)

The Lippmann–Schwinger equation

$$(\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \boldsymbol{\Gamma}_0[\boldsymbol{\tau}] = \bar{\boldsymbol{\epsilon}}$$

Variational form of the Lippmann–Schwinger equation

Find $\boldsymbol{\tau}$ such that $\langle \boldsymbol{\varpi} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} \rangle + \langle \boldsymbol{\varpi} : \boldsymbol{\Gamma}_0[\boldsymbol{\tau}] \rangle = \langle \bar{\boldsymbol{\epsilon}} : \boldsymbol{\varpi} \rangle$ for all $\boldsymbol{\varpi}$

The functional of Hashin–Shtrikman

$$\text{HS}(\boldsymbol{\varpi}; \bar{\boldsymbol{\epsilon}}) = \frac{1}{2} \bar{\boldsymbol{\epsilon}} : \mathbf{C}_0 : \bar{\boldsymbol{\epsilon}} + \langle \bar{\boldsymbol{\epsilon}} : \boldsymbol{\varpi} \rangle - \frac{1}{2} \langle \boldsymbol{\varpi} : (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\varpi} \rangle - \frac{1}{2} \langle \boldsymbol{\varpi} : \boldsymbol{\Gamma}_0[\boldsymbol{\varpi}] \rangle$$

Hashin & Shtrikman, Jmps 10(4), 1962

Willis, Jmps 25(3), 1977

The Hashin–Shtrikman principle (2/3)

Stationarity principle

Hashin & Shtrikman, Jmps 10(4), 1962
Willis, Jmps 25(3), 1977

$$\text{For } (\mathbf{C} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau} + \Gamma_0[\boldsymbol{\tau}] = \bar{\boldsymbol{\epsilon}}$$

$$\frac{\partial HS}{\partial \boldsymbol{\varpi}}(\boldsymbol{\tau}; \bar{\boldsymbol{\epsilon}}) = \mathbf{0}$$

$$HS(\boldsymbol{\tau}; \bar{\boldsymbol{\epsilon}}) = \frac{1}{2} \bar{\boldsymbol{\epsilon}} : \mathbf{C}^{\text{eff}} : \bar{\boldsymbol{\epsilon}}$$

“Soft” reference material

$$\mathbf{C}_0 \leq \mathbf{C} \text{ everywhere in } \Omega$$

$$\frac{1}{2} \bar{\boldsymbol{\epsilon}} : \mathbf{C}^{\text{eff}} : \bar{\boldsymbol{\epsilon}} \leq HS(\boldsymbol{\varpi}; \bar{\boldsymbol{\epsilon}}) \text{ for all } \boldsymbol{\varpi}$$

“Stiff” reference material

$$\mathbf{C}_0 \geq \mathbf{C} \text{ everywhere in } \Omega$$

$$\frac{1}{2} \bar{\boldsymbol{\epsilon}} : \mathbf{C}^{\text{eff}} : \bar{\boldsymbol{\epsilon}} \geq HS(\boldsymbol{\varpi}; \bar{\boldsymbol{\epsilon}}) \text{ for all } \boldsymbol{\varpi}$$

The Hashin–Shtrikman principle (3/3)

General form of trial stress-polarization

$$\boldsymbol{\tau}(\mathbf{x}) = \mathbf{T}(\mathbf{x}) : \bar{\boldsymbol{\epsilon}}$$

HS is a quadratic form!

$$HS(\boldsymbol{\tau}; \bar{\boldsymbol{\epsilon}}) = HS(\mathbf{T} : \bar{\boldsymbol{\epsilon}}, \bar{\boldsymbol{\epsilon}}) = \frac{1}{2} \bar{\boldsymbol{\epsilon}} : \mathbf{C}^{HS} : \bar{\boldsymbol{\epsilon}}$$

\mathbf{C}^{HS} : estimate or bound on \mathbf{C}^{eff}

Any stress-polarization
is admissible!!!

The problem with bounded domains

Closed-form expressions of the Green operator
are generally not known!!!

Heuristic approach

$$\Gamma_0[\tau] \approx \Gamma_0^\infty[\tau - \chi\langle\tau\rangle]$$

Willis, Jmps 25(3), 1977

Rigorous justification

- ▶ Consider the above relation as the definition of a “modified Green operator”
- ▶ The associated Lippmann–Schwinger equation solves **another, well-posed** and **consistent** corrector problem

Brisard, Sab & Dormieux, Jmps 61(12), 2013

Realization-by-realization applications: bounds on the apparent properties

FFT-based methods (1/2)

Features

- ▶ approximate full-field solver: requires **realizations**
- ▶ dedicated to pixel/voxel geometries: ideally suited to **imaging**
- ▶ periodic boundary conditions
- ▶ arguably more efficient than FEM

[Moulinec & Suquet](#), CMAME 157(1-2), 1998

FFT-based methods revisited

- ▶ **cell-wise constant trial stress-polarization**
- ▶ optimization of functional of H&S leads to linear system
- ▶ (matrix-free) linear system can be solved iteratively

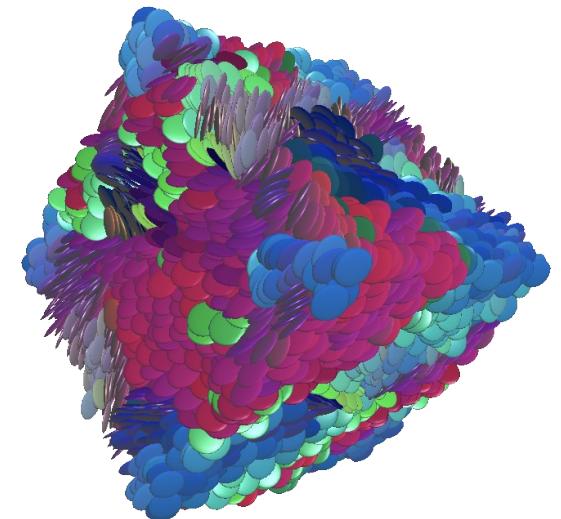
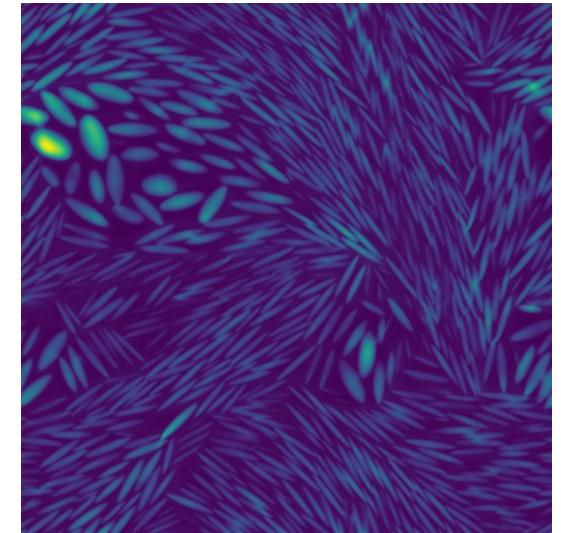
[Brisard & Dormieux](#), Comp. Mat. Sci. 49(3), 2010

[Brisard & Dormieux](#), CMAME 217-220, 2012

FFT-based methods (2/2)

A small, but active community

- ▶ more efficient linear solvers
[Brisard & Dormieux](#), Comp. Mat. Sci. 49(3), 2010
[Zeman et al.](#), J. Comp. Phys. 229(21), 2010
- ▶ improved high-frequency filtering
[Brisard & Dormieux](#), CMAME 217-220, 2012
[Willot](#), CR Mécanique 343(3), 2015
- ▶ error estimates (a priori, a posteriori)
[Schneider](#), Math. Meth. Appl. Sci. 38(13), 2014
[Brisard](#), IJNME 109(4), 2017
- ▶ other discretizations
[Vondřejc et al.](#), CMAME 297, 2015
- ▶ non-linearities (material, geometric)
[Moulinec & Suquet](#), CMAME 157(1-2), 1998
[Gélibart & Mondon-Cancel](#), Comp. Mat. Sci (77), 2013
[Kabel et al.](#), Comp. Mech. 54(6), 2014



Equivalent Inclusion Method (1/2)

Features

- ▶ approximate full-field solver: requires **realizations**
- ▶ dedicated to simple geometries: spheres, ellipsoids
- ▶ **interactions** are explicitly taken into account

[Eshelby](#), Proc. Royal Soc. London A 241(1226), 1957

[Moschovidis & Mura](#), J. App. Mech. 42, 1975

EIM revisited

- ▶ **inclusion-wise polynomial trial stress-polarizations**
- ▶ linear system is small, **but**
- ▶ assembly of the matrix requires off-line (tricky) calculations

[Brisard, Sab & Dormieux](#), JMPS 61(12), 2013

[Brisard, Dormieux & Sab](#), IJSS 51(3-4), 2014

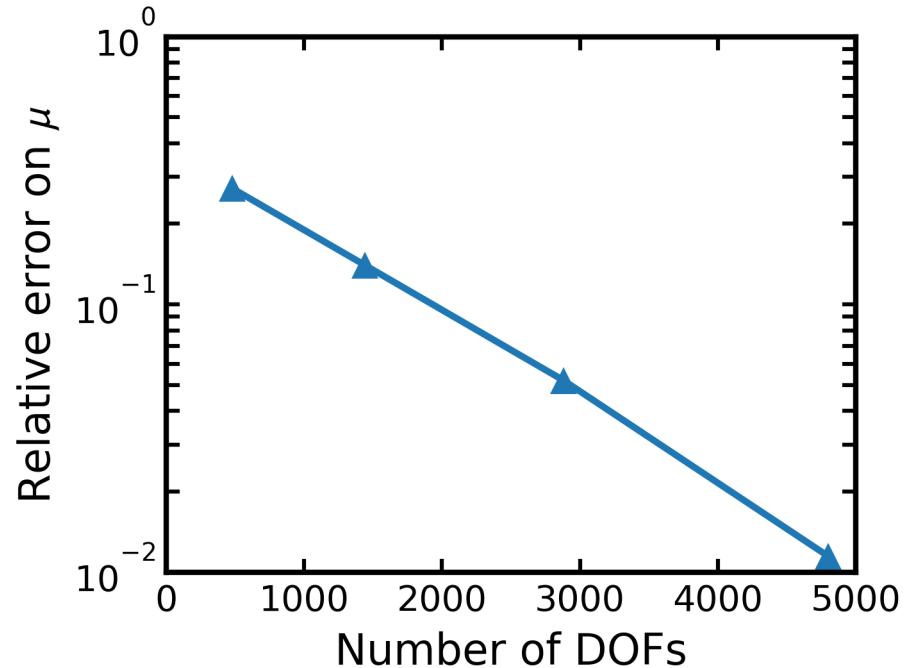
Equivalent Inclusion Method (2/2)

2D (plane strain) application

- ▶ **160 monosized pores**
- ▶ porosity: 40%
- ▶ average over 1000 realizations

**Computation provides
upper-bounds on μ^{eff}**

Degree	Number of DOFs
0	480
1	1440
2	2880
3	4800
FEM	$\approx 320,000$



- ▶ **Exponential convergence!**
- ▶ **Not so good in 3D**

Statistical applications (1/2)

The classical Hashin–Shtrikman bounds

Outline of the statistical approach

1. Pick a (random) trial stress-polarization field

- ▶ $\tau(x, \omega)$ defined over whole space. ω : realization of random material.

2. Apply the Hashin–Shtrikman principle to a finite size “SVE”

- ▶ $\frac{1}{2}\bar{\epsilon} : \mathbf{C}^{\text{app}}(\omega) : \bar{\epsilon} \leq \text{HS}(\chi \tau(\cdot, \omega); \bar{\epsilon})$ χ : indicator function of SVE Ω .

3. Take the ensemble average over all SVEs of given size

- ▶ $\frac{1}{2}\bar{\epsilon} : E[\mathbf{C}^{\text{app}}] : \bar{\epsilon} \leq E[\text{HS}(\chi \tau; \bar{\epsilon})]$

4. Take the limit for large SVEs

- ▶ $\frac{1}{2}\bar{\epsilon} : \mathbf{C}^{\text{eff}} : \bar{\epsilon} \leq \lim_{|\Omega| \rightarrow \infty} E[\text{HS}(\chi \tau; \bar{\epsilon})]$

Willis, Jmps 25(3), 1977

What should we expect?

$$\frac{1}{2} \bar{\epsilon} : \mathbf{C}^{\text{eff}} : \bar{\epsilon} \leq \lim_{|\Omega| \rightarrow \infty} E[\text{HS}(\chi \tau; \bar{\epsilon})]$$

$$\text{HS}(\tau; \bar{\epsilon}) = \frac{1}{2} \bar{\epsilon} : \mathbf{C}_0 : \bar{\epsilon} + \langle \bar{\epsilon} : \tau \rangle - \frac{1}{2} \langle \tau : (\mathbf{C} - \mathbf{C}_0)^{-1} : \tau \rangle - \frac{1}{2} \langle \tau : \Gamma_0[\tau] \rangle$$

One-point information

$$\langle \tau : (\mathbf{C} - \mathbf{C}_0)^{-1} : \tau \rangle = \frac{1}{V} \int_{\mathbf{x} \in \Omega} \tau(\mathbf{x}) : [\mathbf{C}(\mathbf{x}) - \mathbf{C}_0] : \tau(\mathbf{x}) dV_{\mathbf{x}}$$

Two-point information: correlations!

$$\langle \tau : \Gamma_0[\tau] \rangle = \frac{1}{V} \int_{\mathbf{x}, \mathbf{y} \in \Omega} \tau(\mathbf{x}) : \Gamma_0(\mathbf{x}, \mathbf{y}) : \tau(\mathbf{y}) dV_{\mathbf{x}} dV_{\mathbf{y}}$$

Trial stress-polarization

Phase-wise constant trial stress-polarization

$$\boldsymbol{\tau}(\mathbf{x}, \omega) = \sum_{\alpha} \chi_{\alpha}(\mathbf{x}, \omega) \boldsymbol{\tau}_{\alpha}$$

Hashin & Shtrikman, Jmps 10(4), 1962
Willis, Jmps 25(3), 1977

Essential assumption: $\boldsymbol{\tau}_{\alpha}$ constant and deterministic

“Thermodynamic limit” of Hashin–Shtrikman functional

$$\lim_{|\Omega| \rightarrow \infty} E[HS(\chi \boldsymbol{\tau}(\cdot, \omega); \bar{\epsilon})] = \frac{1}{2} \bar{\epsilon} : \mathbf{C}_0 : \bar{\epsilon} + \sum_{\alpha} f_{\alpha} \boldsymbol{\tau}_{\alpha} : \bar{\epsilon} - \frac{1}{2} \sum_{\alpha} f_{\alpha} \boldsymbol{\tau}_{\alpha} : (\mathbf{C}_{\alpha} - \mathbf{C}_0)^{-1} : \boldsymbol{\tau}_{\alpha} - \frac{1}{2} \sum_{\alpha, \beta} \boldsymbol{\tau}_{\alpha} : \mathbf{P}_{\alpha \beta} : \boldsymbol{\tau}_{\beta}$$

Optimization with respect to the $\boldsymbol{\tau}_{\alpha}$ delivers the classical Hashin–Shtrikman bounds

The P-tensors

General expression (proof not so trivial!)

$$\mathbf{P}_{\alpha\beta} = \hat{\mathbf{S}}_{\alpha\beta}(\mathbf{0})\mathbf{P}_0 + \lim_{\delta \rightarrow 0} \int_{\|\mathbf{r}\| \geq \delta} \hat{\mathbf{S}}_{\alpha\beta}(\mathbf{r}) \Gamma_0^\infty(\mathbf{r}) dV_r$$

\mathbf{P}_0 : Hill tensor of spheres

Two-point correlation function (covariance)

$$S_{\alpha\beta}(\mathbf{r}) = E[\chi_\alpha(\mathbf{0})\chi_\beta(\mathbf{r})]$$

$$\hat{\mathbf{S}}_{\alpha\beta}(\mathbf{r}) = S_{\alpha\beta}(\mathbf{r}) - f_\alpha f_\beta$$

Hashin–Shtrikman bounds are expected to account for two-point correlations!

The isotropic case

Angular average of Green operator

$$\int_{\|\mathbf{n}\|=1} \Gamma_0^\infty(\mathbf{n}) dS_{\mathbf{n}} = 0$$

The P-tensors

$$\mathbf{P}_{\alpha\beta} = f_\alpha (\delta_{\alpha\beta} - f_\beta) \mathbf{P}_0$$

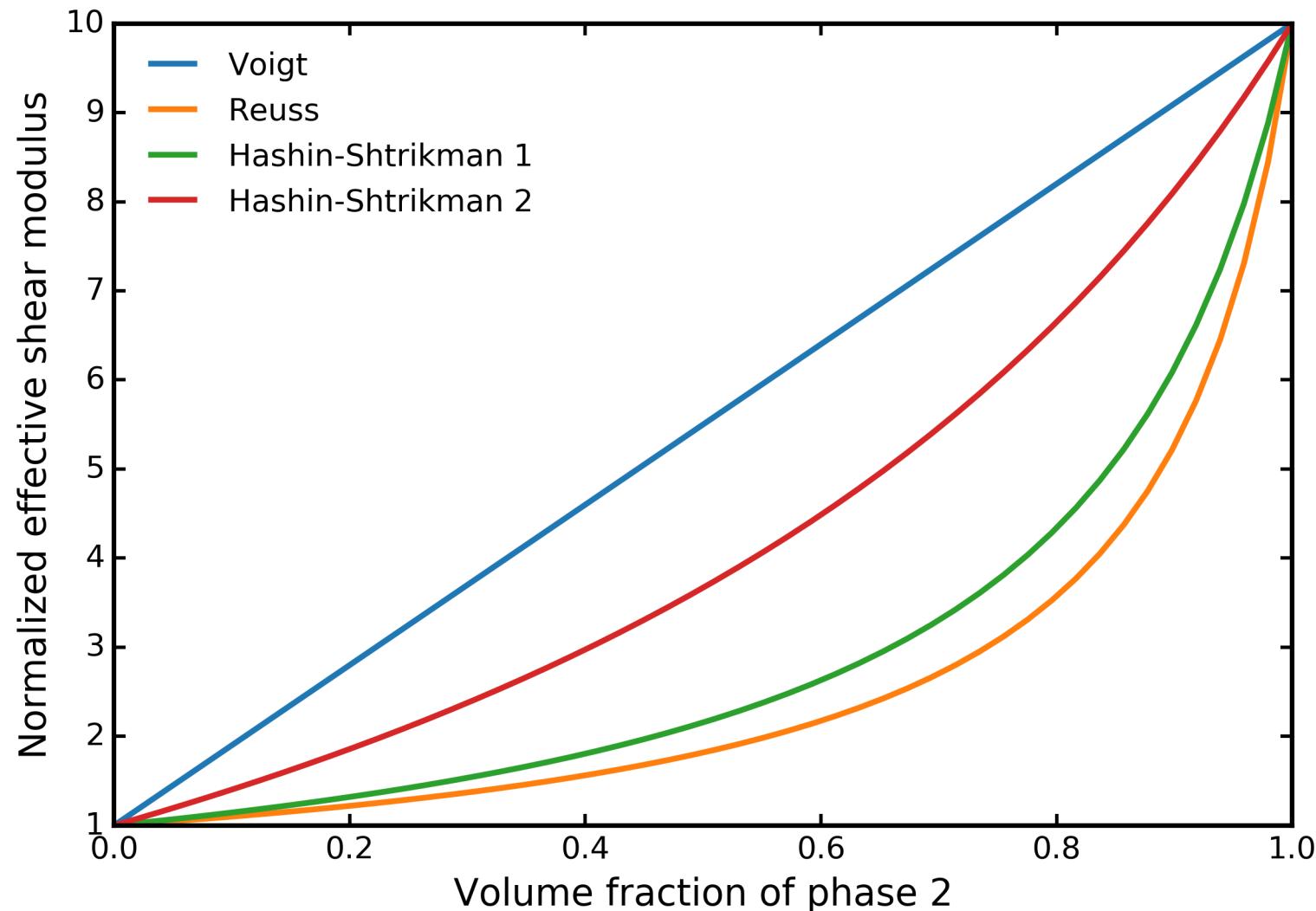
Two-point information is lost!

Expression of the classical bounds

$$\mathbf{C}^{\text{eff}} \leq \mathbf{C}^{\text{HS}} = \sum_{\alpha} f_{\alpha} \mathbf{C}_{\alpha} : \mathbf{A}_{\alpha}^{\text{HS}} \quad \mathbf{A}_{\alpha}^{\text{HS}} = \mathbf{A}_{\alpha}^{\infty} : \left(\sum_{\beta} f_{\beta} \mathbf{A}_{\beta}^{\infty} \right)^{-1} \quad \mathbf{A}_{\alpha}^{\infty} = [\mathbf{I} + \mathbf{P}_0 : (\mathbf{C}_{\alpha} - \mathbf{C}_0)]^{-1}$$

Hashin–Shtrikman bounds account for
volume fractions only!

Hashin–Shtrikman vs. Voigt & Reuss



Statistical applications (2/2)

Towards improved Hashin–Shtrikman bounds?

Probes and statistical descriptors

Reminder: Hashin–Shtrikman trial stress-polarization

$$\boldsymbol{\tau}(\mathbf{x}, \omega) = \sum_{\alpha} \chi_{\alpha}(\mathbf{x}, \omega) \boldsymbol{\tau}_{\alpha}$$

- ▶ χ_{α} will be called a “probe” of the microstructure.

After optimization

- ▶ The resulting bounds depend on f_{α} only.
- ▶ f_{α} will be called a “statistical descriptor” of the microstructure.

χ_{α} is probably a very poor probe!

Enriched trial fields

Abstraction of the classical HS trial fields

$$\begin{aligned}\tau(\mathbf{x}, \omega) &= \sum_{\alpha} \chi_{\alpha}(\mathbf{x}, \omega) \tau_{\alpha} \\ &= \sum_p \text{Probe}_p(\mathbf{x}, \omega) \times \text{Deterministic const.}_p\end{aligned}$$

Introducing new, general probes

$$\tau(\mathbf{x}, \omega) = \sum_{\alpha} \sum_p \chi_{\alpha}(\mathbf{x}, \omega) \psi_p(\mathbf{x}, \omega) \tau_{\alpha p}$$

- ▶ ψ_0, \dots, ψ_M : new probes (not yet specified).
- ▶ $\psi_0 \equiv 1$: ensures that we effectively enrich the classical approach.

Limit of Hashin–Shtrikman functional

$$\lim_{|\Omega| \rightarrow \infty} E[HS(\chi \tau(\cdot, \omega); \bar{\epsilon})] =$$
$$\frac{1}{2} \bar{\epsilon} : \mathbf{C}_0 : \bar{\epsilon} + \sum_{\alpha, p} \Psi_{\alpha p} \tau_{\alpha p} : \bar{\epsilon} - \frac{1}{2} \sum_{\alpha, p, q} \Psi_{\alpha p \alpha q}(\mathbf{0}) \tau_{\alpha p} : (\mathbf{C}_\alpha - \mathbf{C}_0)^{-1} : \tau_{\alpha q}$$
$$- \frac{1}{2} \sum_{\alpha, \beta, p, q} \tau_{\alpha p} : \mathbf{P}_{\alpha p \beta q} : \tau_{\beta q}$$

$$\frac{1}{2} \bar{\epsilon} : \mathbf{C}_0 : \bar{\epsilon} + \sum_{\alpha} f_{\alpha} \tau_{\alpha} : \bar{\epsilon} - \frac{1}{2} \sum_{\alpha} f_{\alpha} \tau_{\alpha} : (\mathbf{C}_\alpha - \mathbf{C}_0)^{-1} : \tau_{\alpha} - \frac{1}{2} \sum_{\alpha, \beta} \tau_{\alpha} : \mathbf{P}_{\alpha \beta} : \tau_{\beta}$$

Enriched statistical descriptors

$$\Psi_{\alpha p} = \mathbb{E}[\chi_\alpha(\mathbf{0}) \psi_p(\mathbf{0})]$$

$$f_\alpha = \mathbb{E}[\chi_\alpha(\mathbf{0})]$$

$$\Psi_{\alpha p \beta q}(\mathbf{r}) = \mathbb{E}[\chi_\alpha(\mathbf{0}) \psi_p(\mathbf{0}) \chi_\beta(\mathbf{r}) \psi_q(\mathbf{r})]$$

$$S_{\alpha\beta}(\mathbf{r}) = \mathbb{E}[\chi_\alpha(\mathbf{0}) \chi_\beta(\mathbf{r})]$$

$$\hat{\Psi}_{\alpha p \beta q}(\mathbf{r}) = \Psi_{\alpha p \beta q}(\mathbf{r}) - \Psi_{\alpha p} \Psi_{\beta q}$$

$$\hat{S}_{\alpha\beta}(\mathbf{r}) = S_{\alpha\beta}(\mathbf{r}) - f_\alpha f_\beta$$

$$\mathbf{P}_{\alpha p \beta q} = \hat{\Psi}_{\alpha p \beta q}(\mathbf{0}) \mathbf{P}_0 + \lim_{\delta \rightarrow 0} \int_{\|\mathbf{r}\| \geq \delta} \hat{\Psi}_{\alpha p \beta q}(\mathbf{r}) \Gamma_0^\infty(\mathbf{r}) dV_r$$

$$\mathbf{P}_{\alpha\beta} = \hat{S}_{\alpha\beta}(\mathbf{0}) \mathbf{P}_0 + \lim_{\delta \rightarrow 0} \int_{\|\mathbf{r}\| \geq \delta} \hat{S}_{\alpha\beta}(\mathbf{r}) \Gamma_0^\infty(\mathbf{r}) dV_r$$

Problem solved?

- ▶ Compute $\Psi_{\alpha p}$ and $\Psi_{\alpha p \beta q}$ (e.g. image analysis)
- ▶ Compute $\mathbf{P}_{\alpha p \beta q}$ (singular integrals)
- ▶ Find the optimum $\tau_{\alpha p}$
- ▶ Evaluate the bound $\frac{1}{2} \bar{\epsilon} : \mathbf{C}^{\text{eff}} : \bar{\epsilon} \leq \lim_{|\Omega| \rightarrow \infty} E[\text{HS}(\chi \tau; \bar{\epsilon})]$

We need to select the probes!

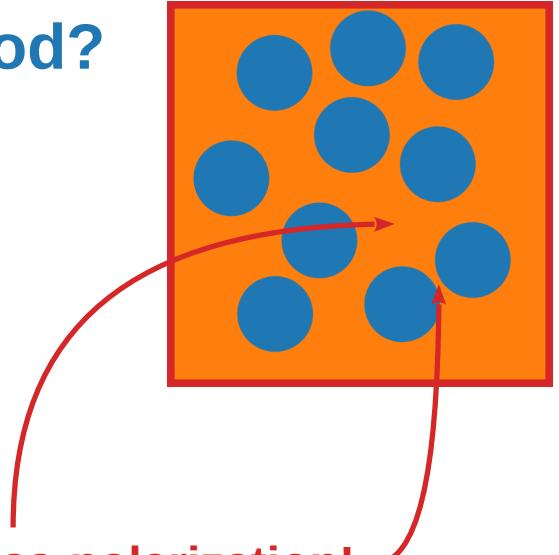
Selecting a probe (1/2)

Why are the classical HS bounds not so good?

$$\boldsymbol{\tau}(\mathbf{x}, \omega) = \sum_{\alpha} \chi_{\alpha}(\mathbf{x}, \omega) \boldsymbol{\tau}_{\alpha}$$

- ▶ Depends on phase at point only.
- ▶ Does not account for neighborhood.

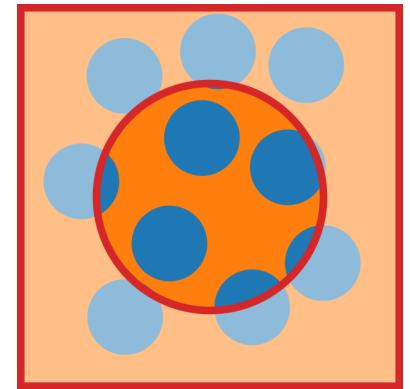
Same trial stress-polarization!



Local volume fraction

- ▶ Accounts for neighborhood!
- ▶ Introduces a length-scale!

$$f_{\alpha}^{\text{loc}}(\mathbf{x}, \omega) = \frac{1}{W} \int w(\mathbf{y} - \mathbf{x}) \chi_{\alpha}(\mathbf{x}, \omega) dV_y$$



Selecting a probe (2/2)

Polynomial expansion

$$\psi_{\alpha p}(\mathbf{x}, \omega) = [f_{\alpha}^{\text{loc}}(\mathbf{x}, \omega)]^p$$

- ▶ Motivated by the $f_{\alpha}(1-f_{\alpha})$ prefactor in classical HS bounds
- ▶ Makes computations tractable.

The case of spherical windows

No improvement on classical HS bounds!

Brisard, Mechanics & Industry 18(2), 2017

Where did we fail?

For isotropic microstructures and spherical windows

$$\Psi_{\alpha p \beta q}(\mathbf{r}) = \Psi_{\alpha p \beta q}(\|\mathbf{r}\|)$$

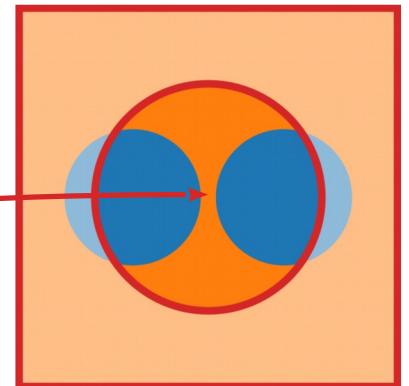
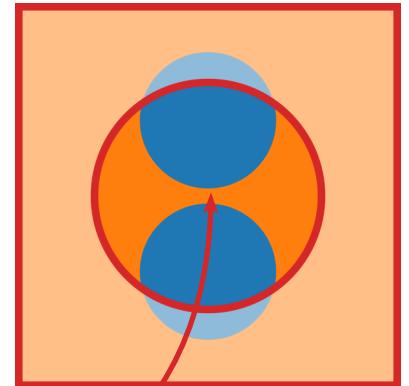
Isotropic probe!

The P-tensors become trivial

$$\begin{aligned} \mathbf{P}_{\alpha p \beta q} &= \hat{\Psi}_{\alpha p \beta q}(\mathbf{0}) \mathbf{P}_0 + \lim_{\delta \rightarrow 0} \int_{\|\mathbf{r}\| \geq \delta} \hat{\Psi}_{\alpha p \beta q}(\|\mathbf{r}\|) \Gamma_0^\infty(\mathbf{r}) dV_r \\ &= \hat{\Psi}_{\alpha p \beta q}(\mathbf{0}) \mathbf{P}_0 \end{aligned}$$

Physical interpretation

Same trial
stress-polarization!

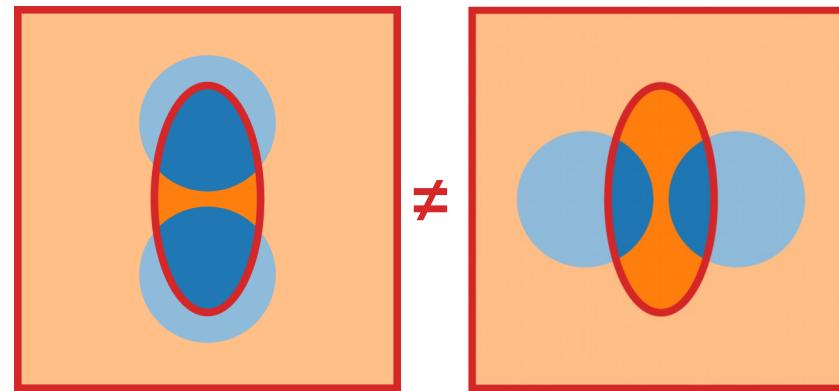


What can be done?

Use anisotropic probes (work in progress)

$\Psi_{\alpha p \beta q}(\mathbf{r})$ must have an angular dependency!

Anisotropic local volume fraction



As a conclusion

Polarization techniques

- ▶ Based on a variational principle
- ▶ No admissibility condition for the trial stress-polarization fields
- ▶ Can provide bounds or estimates of the effective properties
- ▶ Span the whole range of homogenization techniques

The quest for improved bounds

- ▶ Highlights connections between “probes” and stat. descriptors
- ▶ Does not work (yet!)
- ▶ Sheds a new light on the “curse of isotropy”

Perspectives

- ▶ Improved bounds with anisotropic probes
- ▶ Non-linearities (OK for FFT-based methods)

Thank you for your attention!

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