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

Sébastien Brisard

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The Hashin–Shtrikman principle revisited

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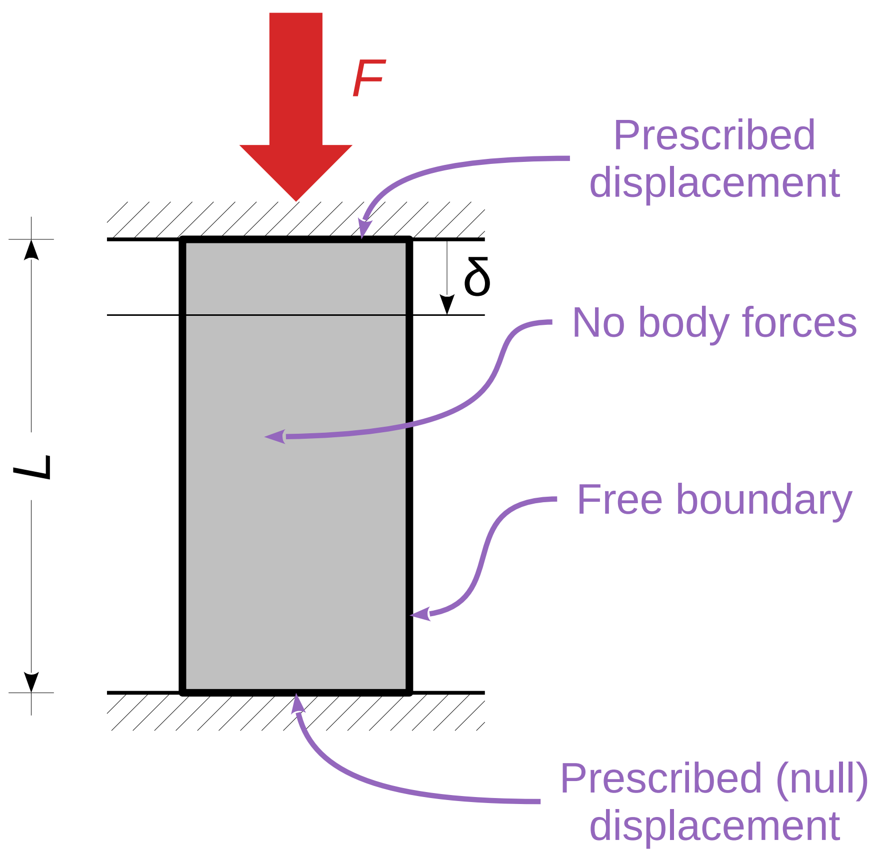
Experimental homogenization

Effective moduli measured through simple uniaxial test

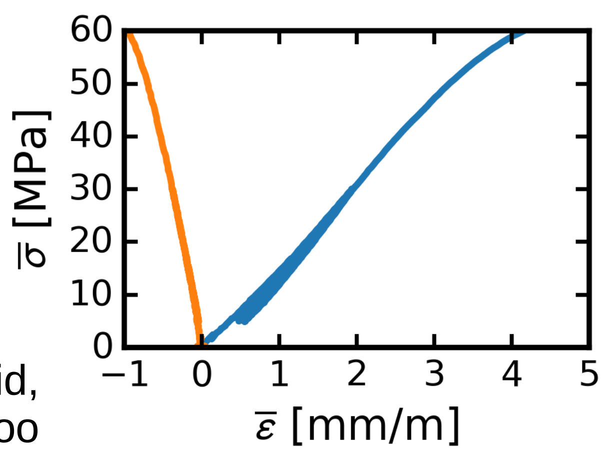


Macroscopic strain & stress

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

Effective Young modulus

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



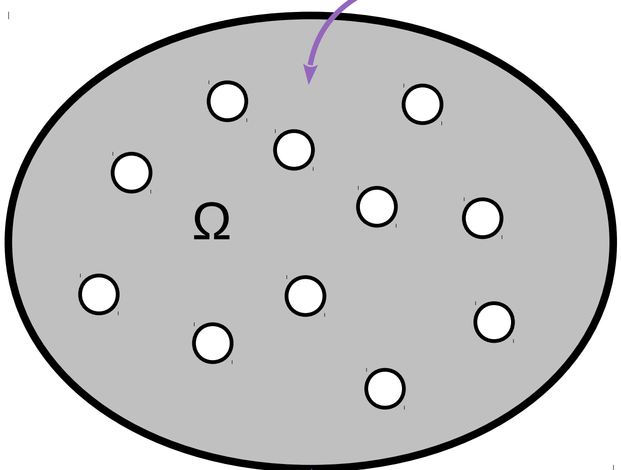
Courtesy S. Bahafid, S. Ghabezloo

Loading conditions are such that

$$\bar{\epsilon} = \langle \epsilon \rangle \qquad \bar{\sigma} = \langle \sigma \rangle \qquad \bar{\sigma}\,\bar{\epsilon} = \langle \sigma\,\epsilon \rangle$$

Numerical homogenization

The corrector problem



No body forces

Imposed displacement

Field equations (in Ω)

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

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

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

Boundary conditions (on ∂Ω)

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

BCs ensure that

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

$$\langle\sigma : \epsilon\rangle = \langle\sigma\rangle : \langle\epsilon\rangle$$

Effective moduli

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

The homogenization toolkit

Pros

- ✔ Simple
- ✔ Versatile

Cons

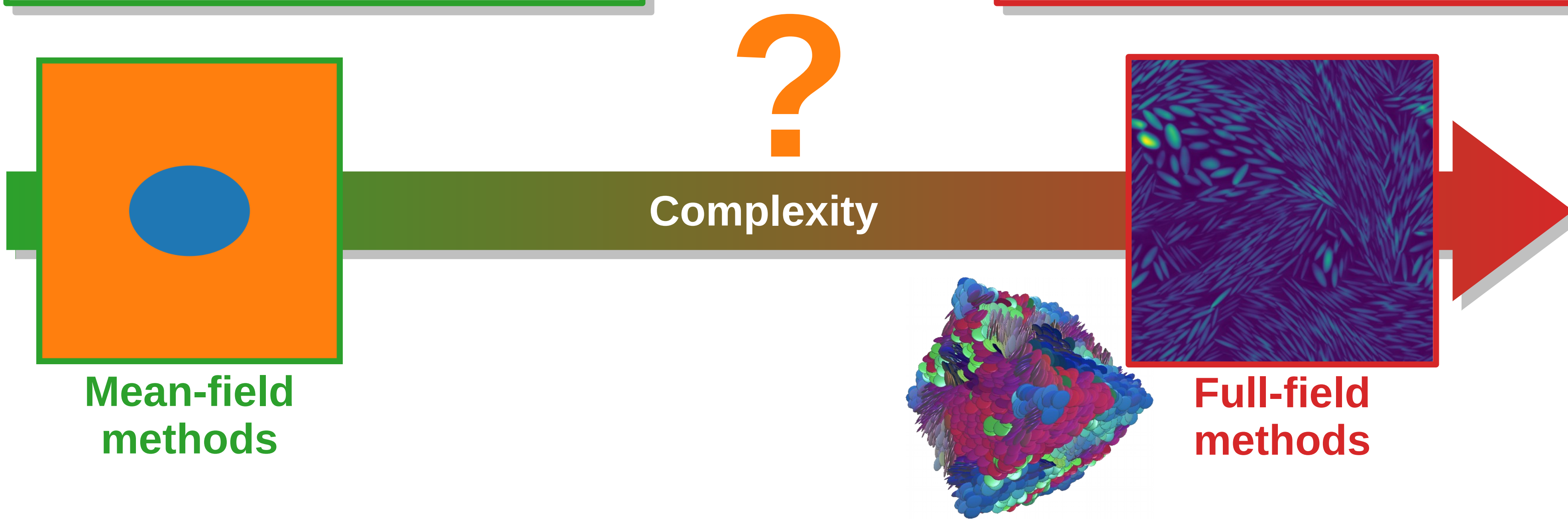
- ✗ No correlations
- ✗ Restricted to ellipsoids!

Pros

- ✔ Captures fine details of microstructure

Cons

- ✗ Time consuming
- ✗ Difficult to analyze



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

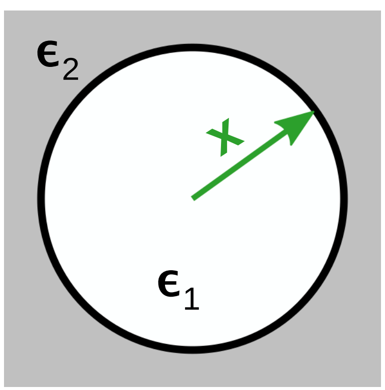
$$\Pi(\boldsymbol{\epsilon}) = \frac{1}{2}\langle \boldsymbol{\epsilon} : \mathbf{C} : \boldsymbol{\epsilon} \rangle \geq \frac{1}{2} \bar{\boldsymbol{\epsilon}} : \mathbf{C}^{\mathrm{eff}} : \bar{\boldsymbol{\epsilon}}$$

Admissible trial strain

In Ω: $\boldsymbol{\epsilon} = \mathbf{sym\,grad\,u}$

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!!!

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

Minimum of complementary energy

Complementary energy

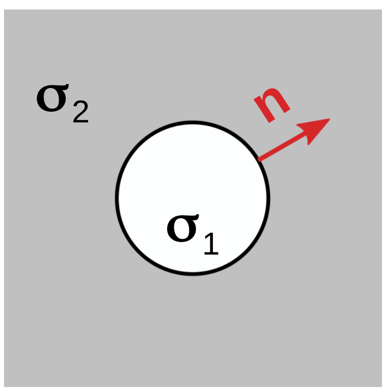
$$\Pi^*(\boldsymbol{\sigma}) = \frac{1}{2}\langle \boldsymbol{\sigma} : \mathbf{S} : \boldsymbol{\sigma}\rangle \geq \frac{1}{2}\bar{\boldsymbol{\sigma}} : \mathbf{S}^{\mathrm{eff}} : \bar{\boldsymbol{\sigma}}$$

Admissible trial stress

In Ω: $\mathbf{div}\,\boldsymbol{\sigma} = \mathbf{0}$

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

Simple admissible trial stress?



- Try phase-wise constant stresses

  $\boldsymbol{\sigma}(\mathbf{x}) = \boldsymbol{\sigma}_\alpha$ for $\mathbf{x}$ in phase α

- Traction is continuous

  $\boldsymbol{\sigma}_1\cdot\mathbf{n} = \boldsymbol{\sigma}_2\cdot\mathbf{n}$ on the interface

Constant trial stress!!!

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

Polarization techniques for homogenization

The Green operator for strains

The initial, corrector problem

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

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

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

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

A new, auxiliary problem

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

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

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

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

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

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

Korringa, J. Math. Phys. 14(4), 1973
Zeller & Dederichs, Physica Status Solidi (B) 55(2), 1973

The Lippmann–Schwinger equation

The initial problem

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

$\Longleftrightarrow$

Introducing the stress-polarization

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

By definition of the Green operator

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

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

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

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

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

Variational form of the Lippmann–Schwinger equation

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

The functional of Hashin–Shtrikman

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

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

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

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

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

“Soft” reference material

$\mathbf{C}_0\leq\mathbf{C}$ everywhere in Ω

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

“Stiff” reference material

$\mathbf{C}_0\geq\mathbf{C}$ everywhere in Ω

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

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!

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

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

Any stress-polarization is admissible!!!

The problem with bounded domains

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

Heuristic approach

$$\boldsymbol{\Gamma}_0[\boldsymbol{\tau}] \simeq \boldsymbol{\Gamma}_0^{\infty}[\boldsymbol{\tau} - \chi \langle \boldsymbol{\tau} \rangle]$$

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

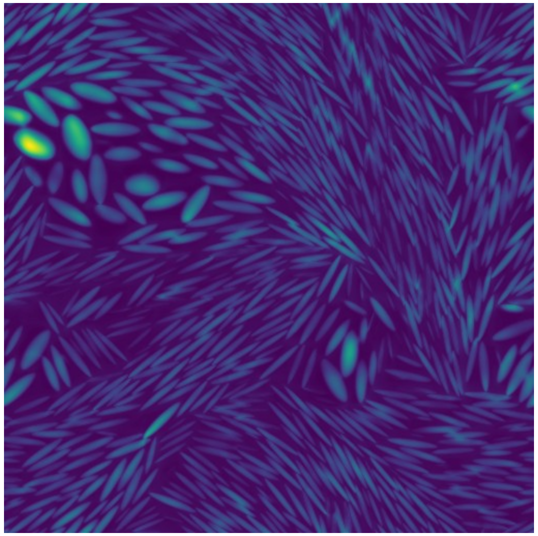
Moulinec & Suquet, CMAME 157(1-2), 1998

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

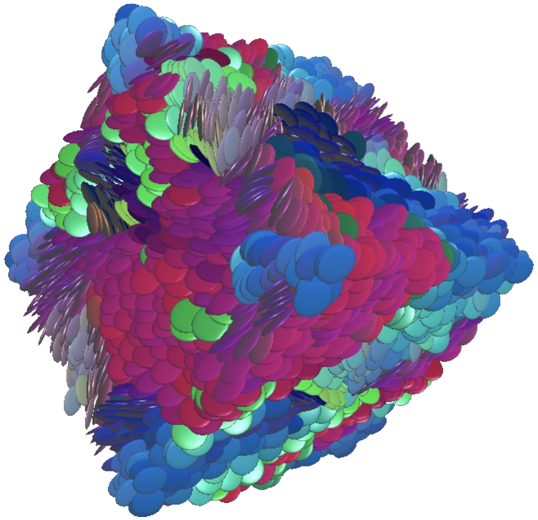
Brisard & Dormieux, Comp. Mat. Sci. 49(3), 2010
Brisard & Dormieux, CMAME 217-220, 2012

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
  Gélébart & 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

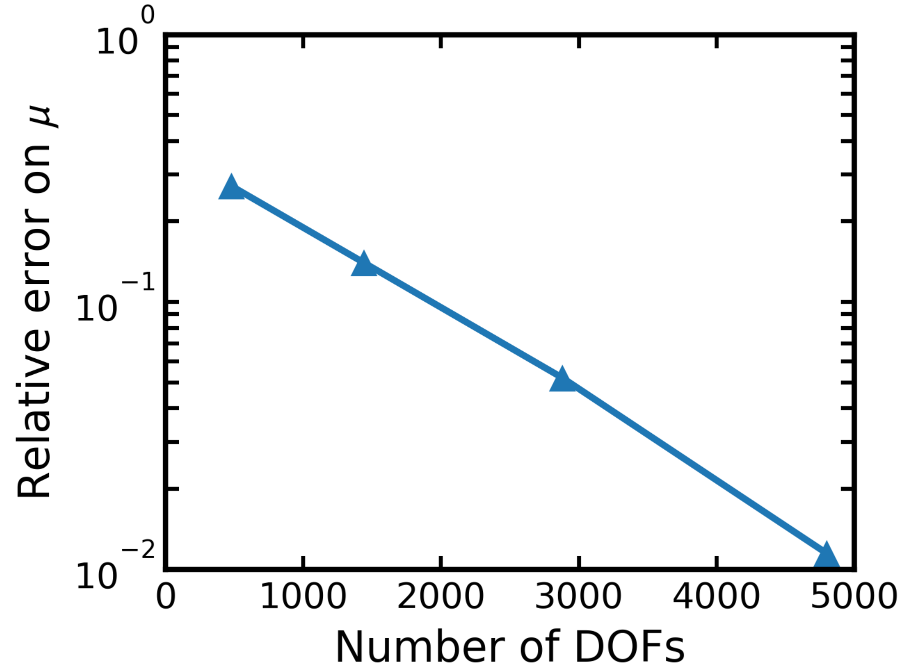
Equivalent Inclusion Method (2/2)

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	≈ 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

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

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

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

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

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

4. Take the limit for large SVEs

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

Willis, JMPS 25(3), 1977

What should we expect?

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

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

One-point information

$$\langle\boldsymbol{\tau}:\left(\mathbf{C}-\mathbf{C}_0\right)^{-1}:\boldsymbol{\tau}\rangle=\frac{1}{V}\int_{\mathbf{x}\in\Omega}\boldsymbol{\tau}(\mathbf{x}):\left[\mathbf{C}(\mathbf{x})-\mathbf{C}_0\right]:\boldsymbol{\tau}(\mathbf{x})\,\mathrm{d}V_{\mathbf{x}}$$

Two-point information: correlations!

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

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

$$\lim_{|\Omega|\to\infty}\mathrm{E}\left[\mathrm{HS}\left(\chi\,\boldsymbol{\tau}(\bullet,\omega);\bar{\boldsymbol{\epsilon}}\right)\right]=$$

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

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

The P-tensors

General expression (proof not so trivial!)

$$\mathbf{P}_{\alpha\beta}=\hat{S}_{\alpha\beta}(\mathbf{0})\mathbf{P}_0+\lim_{\delta\to 0}\int_{\|\mathbf{r}\|\geq\delta}\hat{S}_{\alpha\beta}(\mathbf{r})\,\boldsymbol{\Gamma}_0^{\infty}(\mathbf{r})\,\mathrm{d}V_{\mathbf{r}}$$

$\mathbf{P}_0$: Hill tensor of spheres

Two-point correlation function (covariance)

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

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

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

The isotropic case

Angular average of Green operator

$$\int_{\|\mathbf{n}\|=1} \boldsymbol{\Gamma}_0^\infty(\mathbf{n})\,\mathrm{d}S_{\mathbf{n}} = \mathbf{0}$$

The P-tensors

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

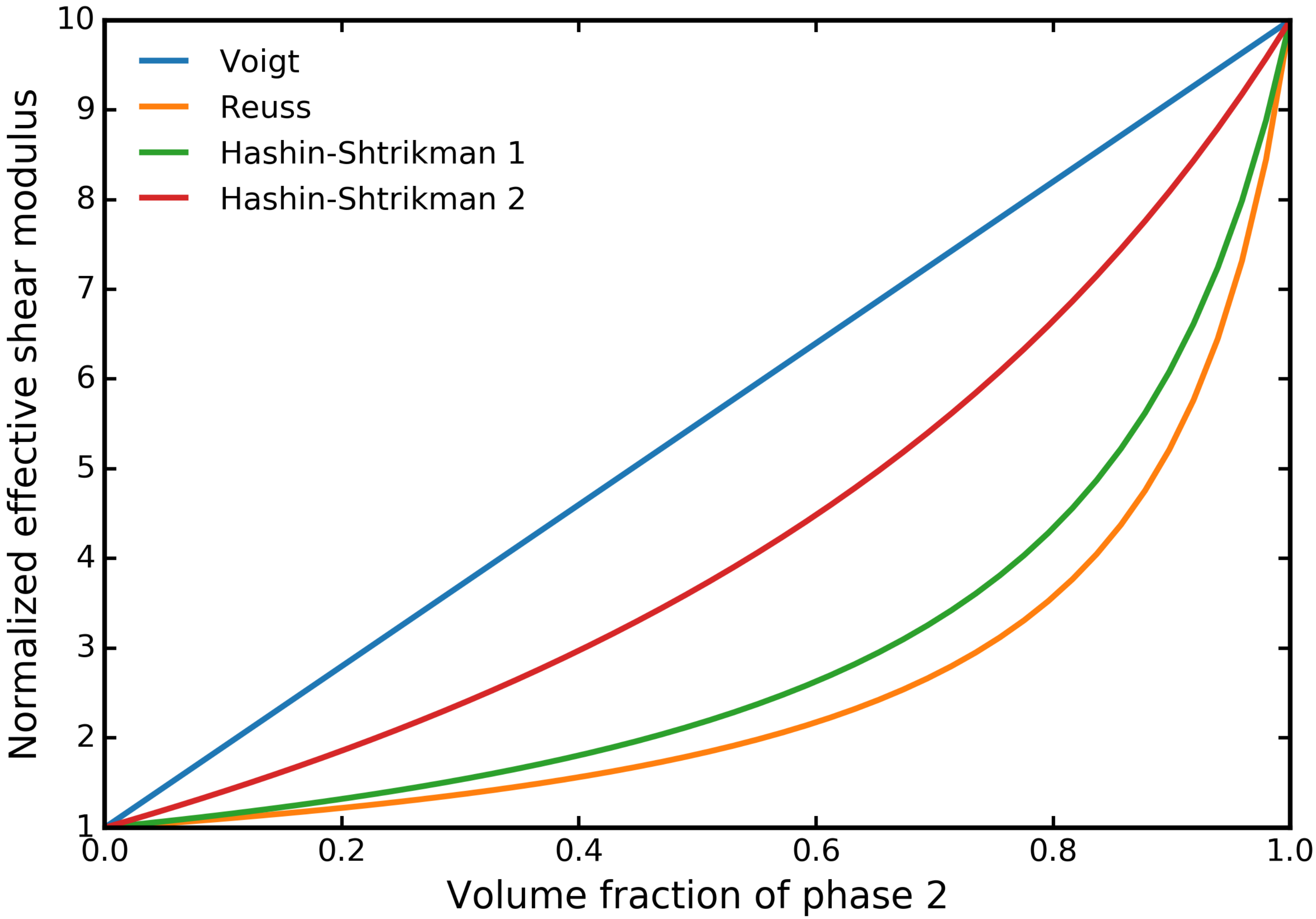
Two-point information is lost!

Expression of the classical bounds

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

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

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

Introducing new, general probes

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

- $\psi_{0,}\ldots,\psi_M$: new probes (not yet specified).
- $\psi_0\equiv 1$: ensures that we effectively enrich the classical approach.

Limit of Hashin–Shtrikman functional

$$\lim_{|\Omega|\to\infty} \mathrm{E}\left[\mathrm{HS}\left(\chi\boldsymbol{\tau}(\bullet,\omega);\bar{\boldsymbol{\epsilon}}\right)\right]=$$

$$\frac{1}{2}\bar{\boldsymbol{\epsilon}}:\mathbf{C}_0:\bar{\boldsymbol{\epsilon}}+\sum_{\alpha,p}\Psi_{\alpha p}\boldsymbol{\tau}_{\alpha p}:\bar{\boldsymbol{\epsilon}}-\frac{1}{2}\sum_{\alpha,p,q}\Psi_{\alpha p\alpha q}(\mathbf{0})\boldsymbol{\tau}_{\alpha p}:\left(\mathbf{C}_\alpha-\mathbf{C}_0\right)^{-1}:\boldsymbol{\tau}_{\alpha q}$$

$$-\frac{1}{2}\sum_{\alpha,\beta,p,q}\boldsymbol{\tau}_{\alpha p}:\mathbf{P}_{\alpha p\beta q}:\boldsymbol{\tau}_{\beta q}$$

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

Enriched statistical descriptors

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

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

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

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

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

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

$$\mathbf{P}_{\alpha p \beta q} = \hat{\Psi}_{\alpha p \beta q}(\mathbf{0})\,\mathbf{P}_0 + \lim_{\delta \to 0} \int_{\|\mathbf{r}\| \geq \delta} \hat{\Psi}_{\alpha p \beta q}(\mathbf{r})\,\mathbf{\Gamma}_0^\infty(\mathbf{r})\,\mathrm{d}V_{\mathbf{r}}$$

$$\mathbf{P}_{\alpha\beta} = \hat{S}_{\alpha\beta}(\mathbf{0})\,\mathbf{P}_0 + \lim_{\delta \to 0} \int_{\|\mathbf{r}\| \geq \delta} \hat{S}_{\alpha\beta}(\mathbf{r})\,\mathbf{\Gamma}_0^\infty(\mathbf{r})\,\mathrm{d}V_{\mathbf{r}}$$

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 $\boldsymbol{\tau}_{\alpha p}$
- Evaluate the bound $\frac{1}{2}\bar{\boldsymbol{\epsilon}}:\mathbf{C}^{\mathrm{eff}}:\bar{\boldsymbol{\epsilon}} \leq \lim_{|\Omega|\rightarrow\infty} \mathrm{E}[\mathrm{HS}(\chi\boldsymbol{\tau};\bar{\boldsymbol{\epsilon}})]$

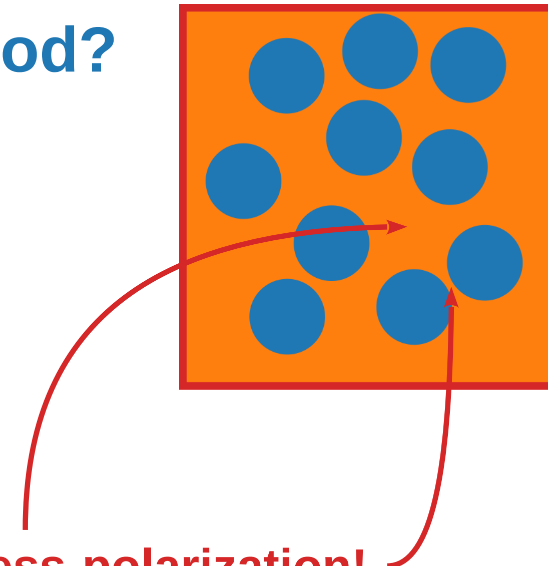
We need to select the probes!

Selecting a probe (1/2)

Why are the classical HS bounds not so good?

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

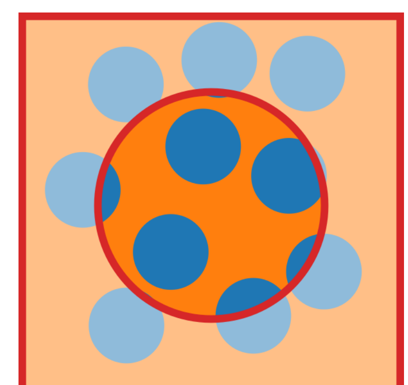
- Depends on phase at point only.
- Does not account for neighborhood.



Local volume fraction

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

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



Selecting a probe (2/2)

Polynomial expansion

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

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

The case of spherical windows

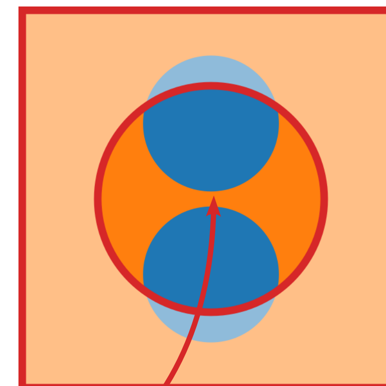
No improvement on classical HS bounds!

Brisard, Mechanics & Industry 18(2), 2017

Where did we fail?

For isotropic microstructures and spherical windows

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



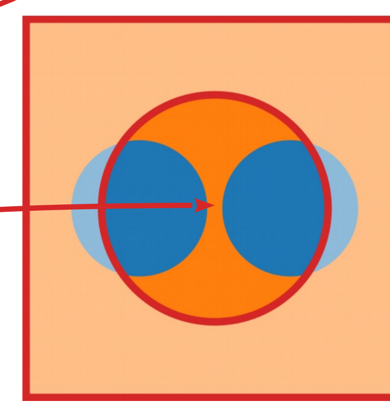
Isotropic probe!

The P-tensors become trivial

$$\begin{aligned}\mathbf{P}_{\alpha p \beta q} &= \hat{\Psi}_{\alpha p \beta q}(\mathbf{0})\mathbf{P}_0 + \lim_{\delta \to 0} \int_{\|\mathbf{r}\| \geq \delta} \hat{\Psi}_{\alpha p \beta q}(\|\mathbf{r}\|)\, \mathbf{\Gamma}_0^\infty(\mathbf{r})\, \mathrm{d}V_{\mathbf{r}} \\ &= \hat{\Psi}_{\alpha p \beta q}(\mathbf{0})\mathbf{P}_0\end{aligned}$$

Physical interpretation

Same trial stress-polarization!

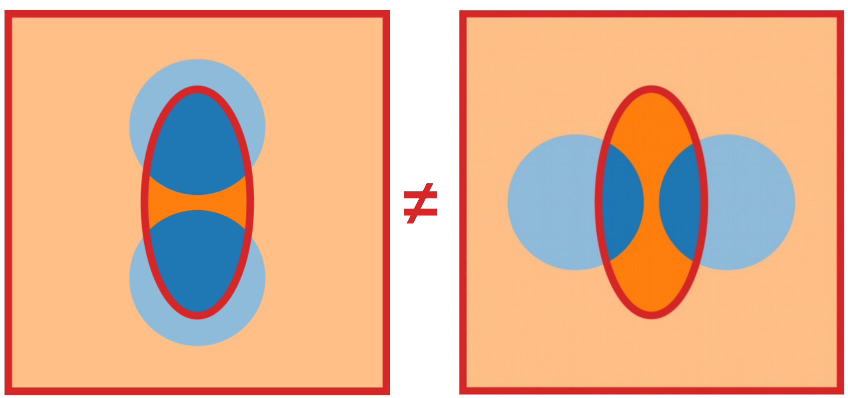


What can be done?

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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