

# Microstructure and mechanical properties

## Polarization techniques to the rescue

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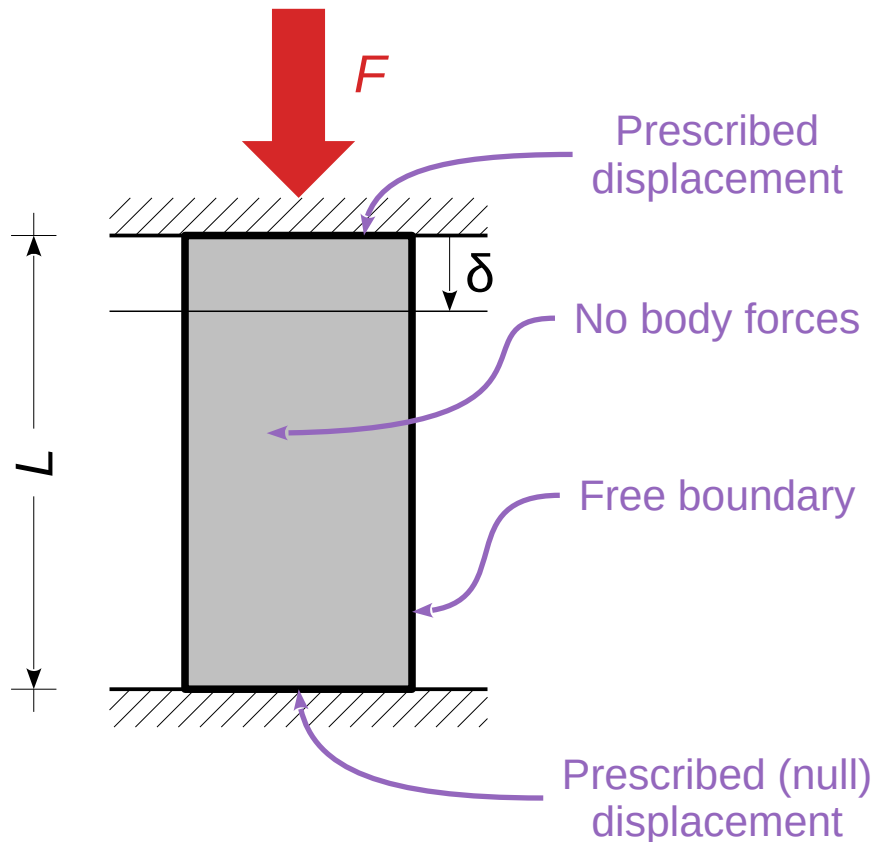


IFSTTAR



# Experimental homogenization

## Effective moduli measured through simple uniaxial test

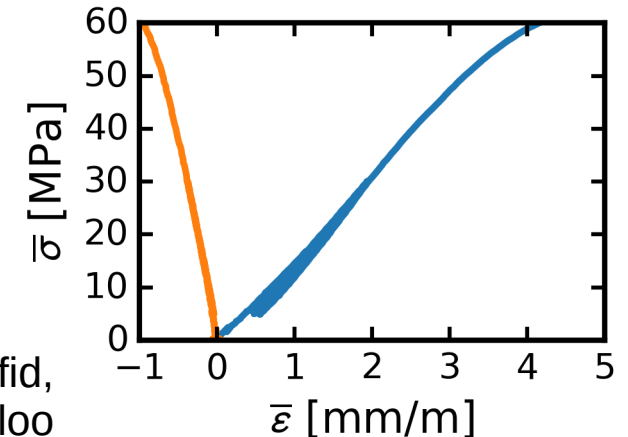


## Macroscopic strain & stress

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

## Effective Young modulus

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



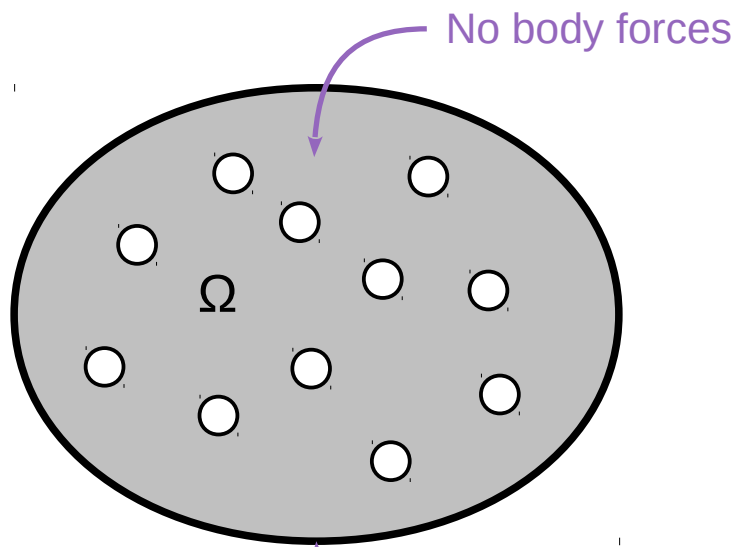
Courtesy S. Bahafid,  
S. Ghabezloo

## 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



### Field equations (in $\Omega$ )

$$\partial_j \sigma_{ij} = 0$$

$$\sigma_{ij} = C_{ijkl} \epsilon_{kl}$$

$$2\epsilon_{ij} = \partial_i u_j + \partial_j u_i$$

### Boundary conditions (on $\partial\Omega$ )

$$u_i(x_j) = \bar{\epsilon}_{ij} x_j$$

### BCs ensure that

$$\langle \epsilon_{ij} \rangle = \bar{\epsilon}_{ij} \quad \langle \sigma_{ij} \epsilon_{ij} \rangle = \langle \sigma_{ij} \rangle \langle \epsilon_{ij} \rangle$$

### Effective moduli

$$\langle \sigma_{ij} \rangle = C_{ijkl}^{\text{eff}} \langle \epsilon_{kl} \rangle$$

# The homogenization toolkit

## Pros

- ✓ Simple
- ✓ Versatile

## Cons

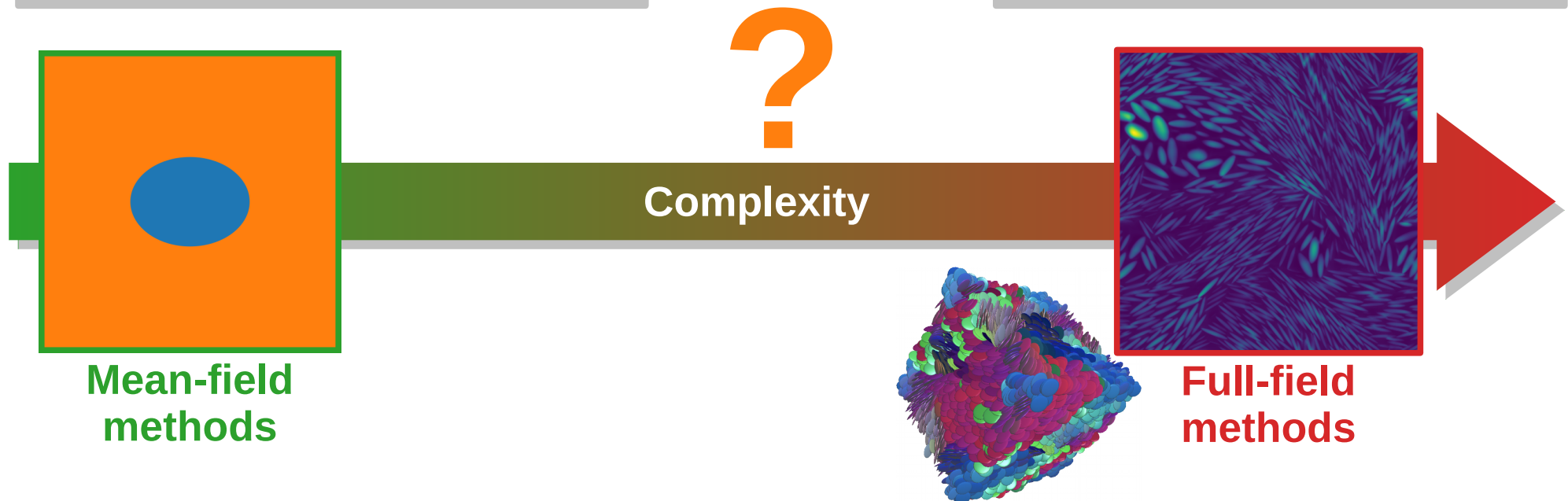
- ✗ No correlations
- ✗ Restricted to ellipsoids!

## Pros

- ✓ Captures fine details of microstructure

## Cons

- ✗ Time consuming
- ✗ Difficult to analyze



# Outline of this talk

## Introducing the principle of Hashin & Shtrikman (H&S)

- ▶ Variational methods for homogenization
- ▶ Potential energy, complementary energy
- ▶ “Energy” of Hashin & Shtrikman

## Going down the complexity scale

- ▶ “FFT-based” method works very well
- ▶ Equivalent inclusion method works quite well
- ▶ Improved H&S bounds does not work (yet?)



# 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?**

# Potential energy

## Potential energy

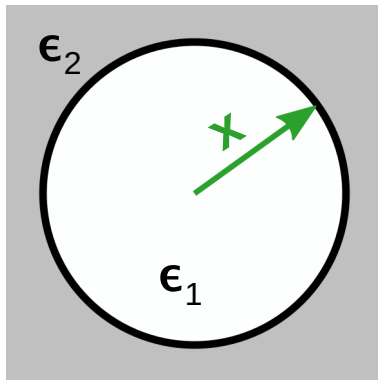
$$W(\boldsymbol{\epsilon}) = \frac{1}{2} \langle \epsilon_{ij} \mathbf{C}_{ijkl} \epsilon_{kl} \rangle \geq \frac{1}{2} \bar{\epsilon}_{ij} \mathbf{C}_{ijkl}^{\text{eff}} \bar{\epsilon}_{kl}$$

## Admissible trial strain

$$\text{In } \Omega: \epsilon_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i)$$

## Simple admissible trial strain?

$$\text{On } \partial\Omega: u_i = \bar{\epsilon}_{ij} X_j$$



- ▶ Try phase-wise constant strains

$$\epsilon_{\alpha,ij} = \text{const.} \Rightarrow u_{\alpha,i}(\mathbf{x}) = \epsilon_{\alpha,ij} X_j$$

- ▶ Displacement is continuous

$$\epsilon_{1,ij} X_j = \epsilon_{2,ij} X_j \text{ on the interface}$$

## Constant strain field!!!

$$\mathbf{C}^{\text{eff}} \leq \langle \mathbf{C} \rangle$$

(Voigt)

# Complementary energy

## Complementary energy

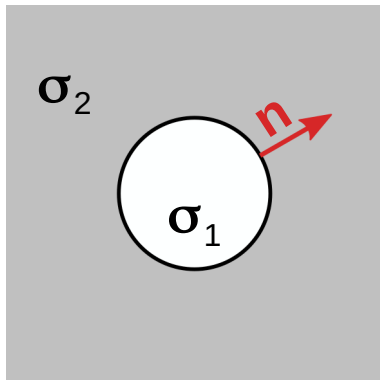
$$W^*(\boldsymbol{\sigma}) = \frac{1}{2} \langle \sigma_{ij} \mathbf{S}_{ijkl} \sigma_{kl} \rangle \geq \frac{1}{2} \bar{\sigma}_{ij} \mathbf{S}_{ijkl}^{\text{eff}} \bar{\sigma}_{kl}$$

## Admissible trial stress

$$\text{In } \Omega: \partial_j \sigma_{ij} = 0$$

## Simple admissible trial stress?

$$\text{On } \partial\Omega: \sigma_{ij} n_j = \bar{\sigma}_{ij} n_j$$



- ▶ Try phase-wise constant stresses

$$\sigma_{\alpha,ij} = \text{const.}$$

- ▶ Traction is continuous

$$\sigma_{1,ij} n_j = \sigma_{2,ij} n_j \text{ on the interface}$$

## Constant trial stress!!!

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



# Principle of Hashin & Shtrikman

$$H(\boldsymbol{\tau}) = \frac{1}{2} \bar{\epsilon}_{ij} \mathbf{C}_{ijkl}^0 \bar{\epsilon}_{kl} + \langle \bar{\epsilon}_{ij} \tau_{ij} \rangle - \frac{1}{2} \langle \tau_{ij} (\mathbf{C} - \mathbf{C}^0)^{-1}_{ijkl} \tau_{kl} \rangle - \frac{1}{2} \langle \tau_{ij} \Gamma_{ijkl}^0 * \tau_{kl} \rangle$$

Stress-polarization

Reference material (user-defined)

Green operator for strains

Convolution product

**H is stationary “at equilibrium”**

$$\frac{\partial H}{\partial \boldsymbol{\tau}} [\boldsymbol{\tau}^{\text{cr}}] = 0 \quad \text{and} \quad H[\boldsymbol{\tau}^{\text{cr}}] = \frac{1}{2} \bar{\epsilon}_{ij} \mathbf{C}_{ijkl}^{\text{eff}} \bar{\epsilon}_{kl}$$

**Extremum principle**

$$\boldsymbol{\tau}_{ij}^{\text{cr}} = (\mathbf{C}_{ijkl} - \mathbf{C}_{ijkl}^0) \epsilon_{kl} \quad \text{True strain}$$

$$\frac{1}{2} \bar{\epsilon}_{ij} \mathbf{C}_{ijkl}^{\text{eff}} \bar{\epsilon}_{kl} \begin{matrix} \leq \\ \geq \end{matrix} H(\boldsymbol{\tau}) \text{ for all } \boldsymbol{\tau}$$

“Soft” ref. mat. (pointing to the upper bound)

“Stiff” ref. mat. (pointing to the lower bound)



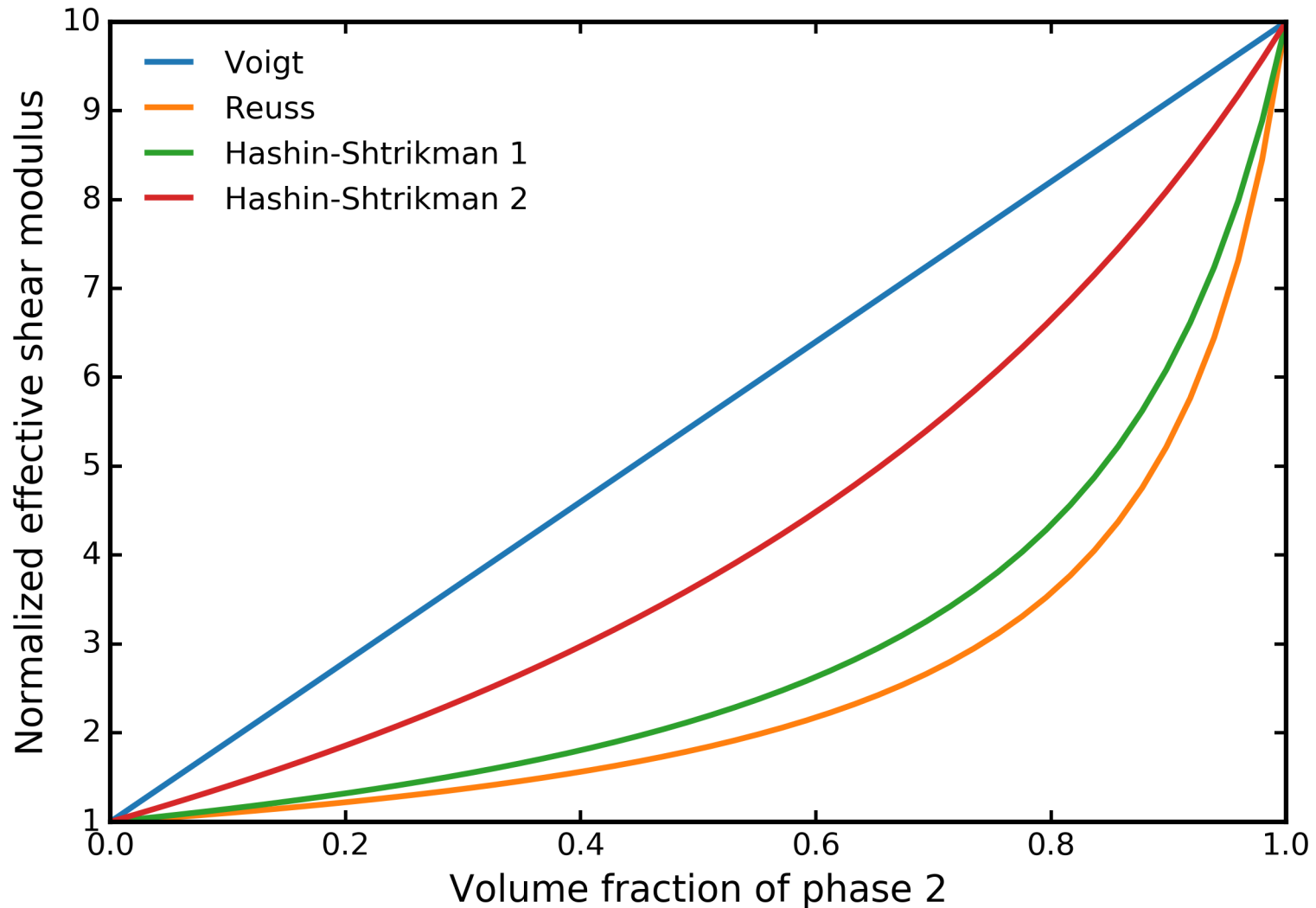
**Any stress-polarization is admissible!!!**



Z. Hashin & S. Shtrikman (1962), *JMPS* 10(4)

# Bounds of Hashin & Shtrikman

## Phase-wise constant trial stress-polarization



# The principle of Hashin & Shtrikman

## New applications

### The classical bounds of Hashin & Shtrikman

The trial stress field is (too) simple

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

Indicator function of phase  $\alpha$  (random)

Constant polarization in phase  $\alpha$  (deterministic)

→ **Enriched trial stress-polarizations?**



# Going down the complexity scale



# Uniform Grid, Periodic Lippmann–Schwinger solvers (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

H. Moulinec & P. Suquet (1998), *CMAME* 157(1-2)

## UGPLS solvers 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

SB & L. Dormieux (2010) *Comp. Mat. Sci.* 49(3)

SB & L. Dormieux (2012) *CMAME* 217-220

# Uniform Grid, Periodic Lippmann-Schwinger solvers (2/2)

## A small, but active community

- ▶ more efficient linear solvers

SB & L. Dormieux (2010), *Comp. Mat. Sci.* **49(3)**

J. Zeman et al. (2010), *J. Comp. Phys.* **229(21)**

- ▶ improved high-frequency filtering

SB & L. Dormieux (2012), *CMAME* **217-220**

F. Willot (2015), *CR Mécanique* **343(3)**

- ▶ error estimates (a priori, a posteriori)

M. Schneider (2014) *Math. Meth. Appl. Sci.* **38(13)**

SB (2017) *IJNME*, 10.1002/nme.5263

- ▶ other discretizations

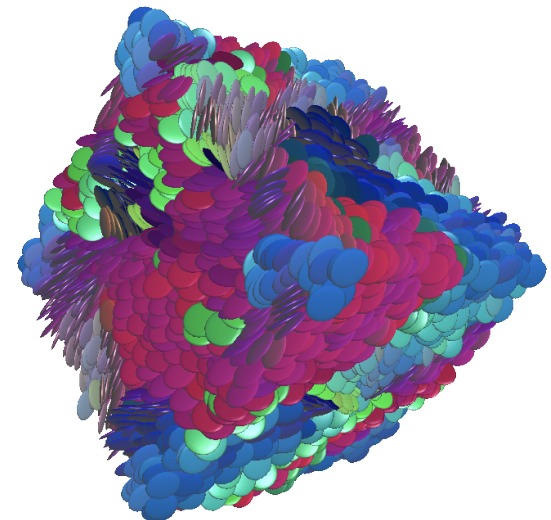
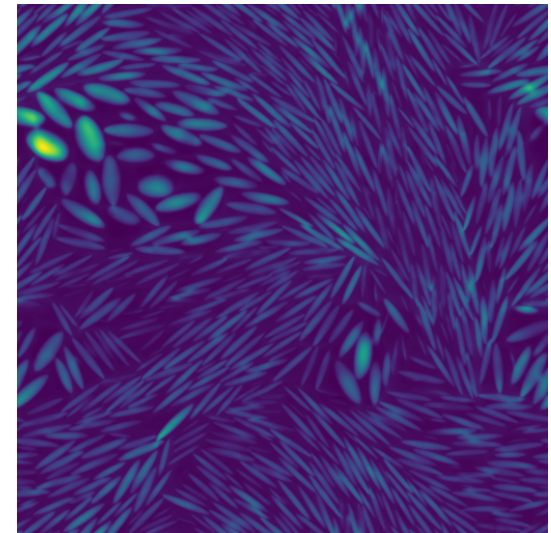
J. Vondřejc et al. (2015) *CMAME* **297**

- ▶ non-linearities (material, geometric)

H. Moulinec & P. Suquet (1998), *CMAME* **157(1-2)**

L. Gélébart & R. Mondon-Cancel (2013), *Comp. Mat. Sci.* **(77)**

M. Kabel et al. (2014) *Comp. Mech.* **54(6)**



# Going down the complexity scale



# Equivalent Inclusion Method (1/2)

## Features

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

Z.A. Moschovidis & T. Mura (1975), *J. App. Mech.* 42

## EIM revisited

- ▶ inclusion-wise polynomial trial stress-polarizations
- ▶ optimization of the functional of Hashin & Shtrikman leads to a linear system
- ▶ linear system is small, **but**
- ▶ assembly of the matrix requires off-line (difficult) calculations

SB, K. Sab & L. Dormieux (2013), *JMPS* 61(12)

SB, L. Dormieux & K. Sab (2014), *IJSS* 51(3-4)

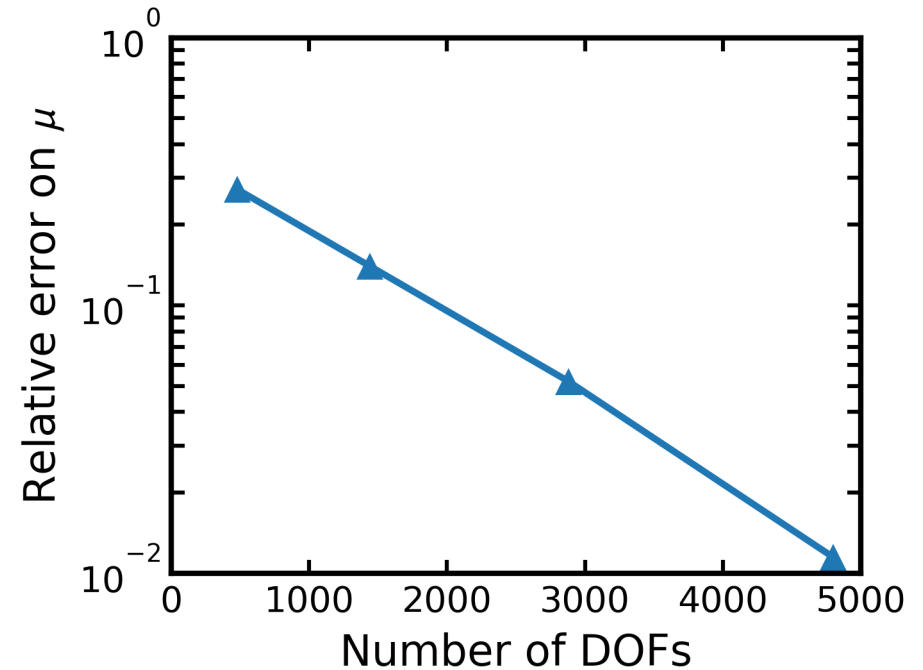


# Equivalent Inclusion Method (2/2)

## 2D (plane strain) application

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

**Computation provides upper-bounds on  $\mu^{\text{eff}}$**



**Degree**      **Number of DOFs**

0              480

1              1440

2              2880

3              4800

FEM               $\approx 320,000$



**Exponential convergence!**



**Not so good in 3D**



# Going down the complexity scale



# Improved bounds (1/2)

## Probes and statistical descriptors

$\boldsymbol{\tau}(\mathbf{x}) = \sum_{\alpha} \chi_{\alpha}(\mathbf{x}) \boldsymbol{\tau}_{\alpha}$  results in bounds that depend on  $f_{\alpha}$

- ▶ probe:  $\chi_{\alpha}$
- ▶ statistical descriptor:  $f_{\alpha}$

## Introducing new probes

To produce bounds that depend on finer statistical descriptors

$$\boldsymbol{\tau}(\mathbf{x}) = \sum_{\alpha} \sum_{\rho} \chi_{\alpha}(\mathbf{x}) \psi_{\rho}(\mathbf{x}) \boldsymbol{\tau}_{\alpha\rho}$$

- ▶ Optimization over **all** realizations
- ▶ Resulting statistical descriptors:  $E[\chi_{\alpha}(\mathbf{0}) \psi_{\rho}(\mathbf{0}) \chi_{\beta}(\mathbf{r}) \psi_{q}(\mathbf{r})]$

# Improved bounds (2/2)

## Probing with local volume fraction

$$\psi_p(\mathbf{x}) = [f^{\text{loc}}(\mathbf{x})]^p$$

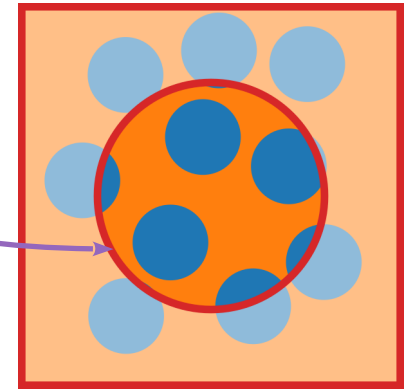


**No improvement on the bounds**

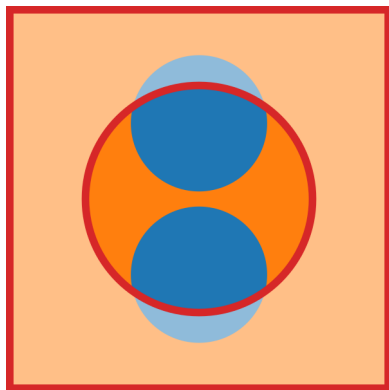
SB (2017), *Mechanics & Industry*, accepted



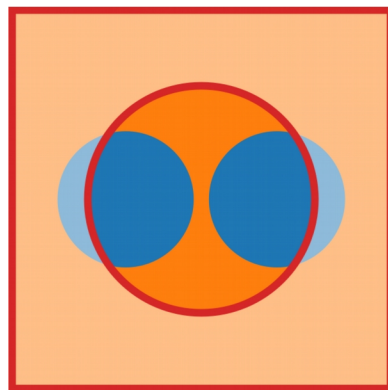
Sliding window



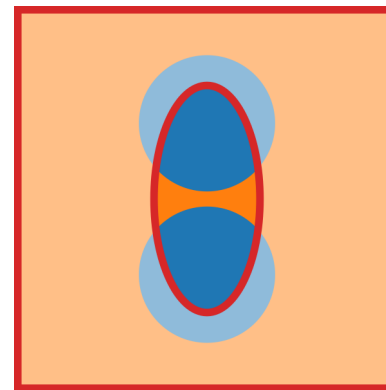
## Isotropic probing vs. anisotropic probing (work in progress)



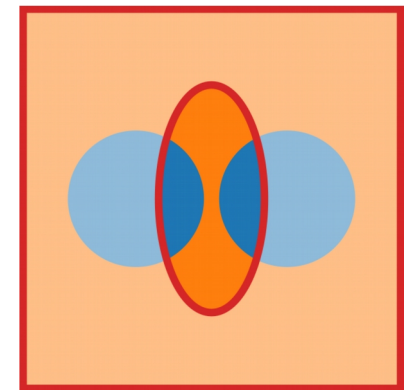
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Isotropic probe



≠



Anisotropic probe

# As a conclusion

## Polarization techniques

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

## Perspectives

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

# Thank you for your attention!

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<http://sbrisard.github.io>



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