



Homogenization-based interpolation of material properties for phase-field models

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Free energy

Decomposition of the free energy

$$f(\phi, \nabla\phi, c, \boldsymbol{\varepsilon}) = f_\phi(\phi, \nabla\phi) + f_c(\phi, c) + f_{\text{el}}(\phi, \boldsymbol{\varepsilon})$$

Contribution of interface

$$f_\phi(\phi, \nabla\phi) = \frac{3\gamma}{\ell} [W(\phi) + \ell^2 \|\nabla\phi\|^2] \quad \text{with} \quad W(\phi) = \phi^2(1 - \phi)^2$$

Chemical & mechanical contributions

$$\begin{cases} f_c(\phi, c) \\ f_{\varepsilon}(\phi, \boldsymbol{\varepsilon}) \end{cases} \quad \text{such that} \quad \begin{cases} f_c(0, c) = f_c^0(c) \\ f_{\varepsilon}(0, \boldsymbol{\varepsilon}) = f_{\varepsilon}^0(\boldsymbol{\varepsilon}) \end{cases} \quad \text{and} \quad \begin{cases} f_c(1, c) = f_c^1(c) \\ f_{\varepsilon}(1, \boldsymbol{\varepsilon}) = f_{\varepsilon}^1(\boldsymbol{\varepsilon}) \end{cases}$$

Properties of the transition zone

- (Fictitious) “mixture” of the two pure phases
- Properties classically interpolated between pure phases [1]
- Voigt/Reuss estimates [2–4] from theory of **generalized standard materials** [5]
- Laminate theory in finite elasticity [6] from variational approach
- Is it possible to introduce more general **homogenization models**?
- What would be the gain?
→ Thermodynamical consistency vs. quality of numerical solution ?

[1] A. G. Khachaturyan, *Theory of Structural Transformations in Solids*, Dover ed, Dover Publications, Mineola, N.Y, 2008.

[2] K. Ammar et al., *European Journal of Computational Mechanics* 2009, 18, 485–523.

[3] K. Ammar, PhD thesis, École Nationale Supérieure des Mines de Paris, 2010.

[4] K. Ammar et al., *Philosophical Magazine Letters* 2011, 91, 164–172.

[5] B. Halphen, Q. Son Nguyen, *Journal de Mécanique* 1975, 14, 39–63.

[6] J. Mosler, O. Shchyglo, H. Montazer Hojjat, *Journal of the Mechanics and Physics of Solids* 2014, 68, 251–266.

Digression: incompressible binary fluids

“Density-matched” fluids

The first case considered [1, 2]. When $\rho_0 = \rho_1$, $\rho(\phi) = \rho_0 = \rho_1$ is suitable and **the mixture is incompressible**: $\nabla \cdot \mathbf{u} = 0$ everywhere.

Fluids with density contrast

$$\rho(\phi) = (1 - \phi)\rho_0 + \phi\rho_1$$

$\nabla \cdot \mathbf{u} = 0$ no longer holds! See refs [3, 4].

Interpolation scheme requires some thinking!

[1] D. Jacqmin, *Journal of Computational Physics* **1999**, 155, 96–127.

[2] V. E. Badalassi, H. D. Ceniceros, S. Banerjee, *Journal of Computational Physics* **2003**, 190, 371–397.

[3] H. Ding, P. D. M. Spelt, C. Shu, *Journal of Computational Physics* **2007**, 226, 2078–2095.

[4] H. Abels, H. Garcke, G. Grün, *Mathematical Models and Methods in Applied Sciences* **2012**, 22, 1150013.

Towards homogenization

- Transition zone as a two-phase, heterogeneous material
- $(1 - \phi)$ and ϕ : “volume fractions” of phases 0 ($\phi = 0$) and 1 ($\phi = 1$)
- Localization: $c \mapsto c_0, c_1$ and $\boldsymbol{\varepsilon} \mapsto \boldsymbol{\varepsilon}_0, \boldsymbol{\varepsilon}_1$
- Only the “macroscopic” variables c and $\boldsymbol{\varepsilon}$ are state variables!
 $(c_0, c_1, \boldsymbol{\varepsilon}_0$ et $\boldsymbol{\varepsilon}_1$ are **not** state variables)

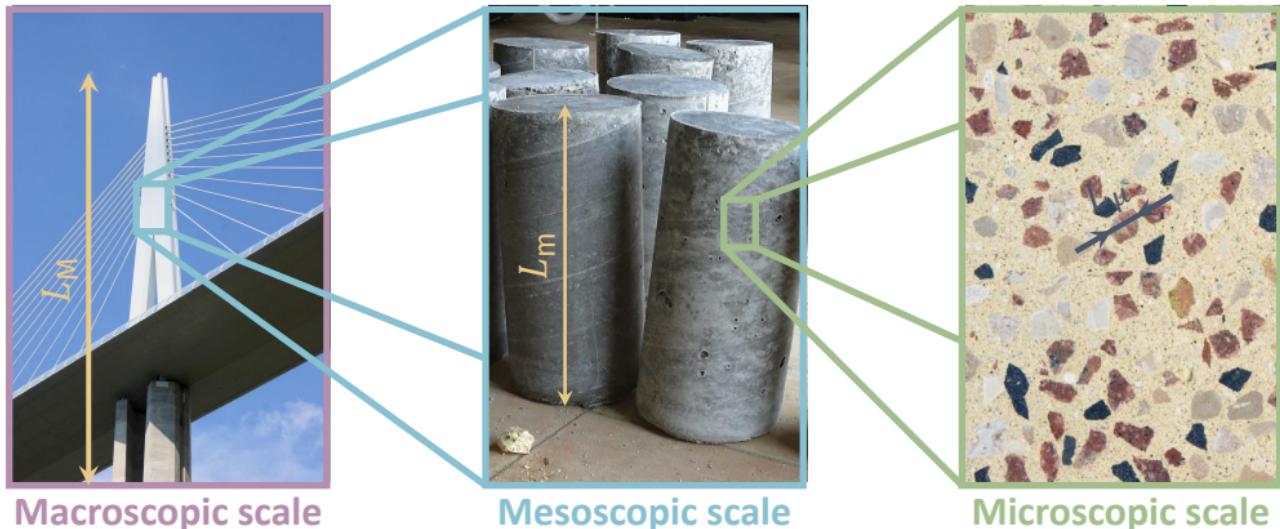
Outline

- A (very brief) overview of random homogenization [1]
- Application to phase-field models

[1] A. Zaoui, *Journal of Engineering Mechanics* **2002**, 128, 808–816.

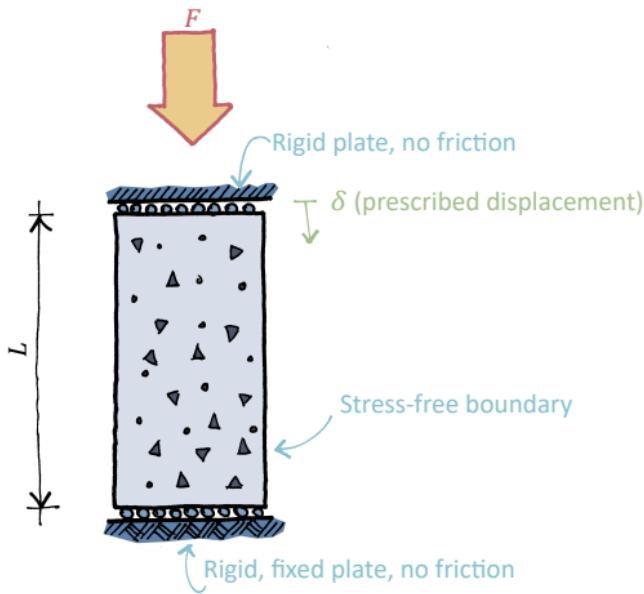
A (very brief) overview of random homogenization

Separation of scales



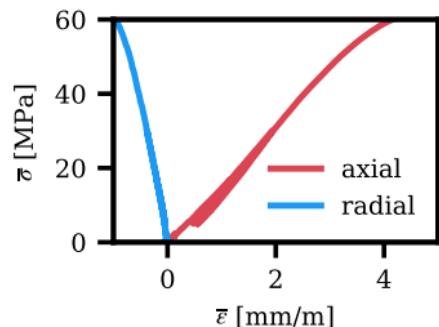
$$L_\mu \ll L_m \ll L_M$$

Top-down (experimental) characterization



Macroscopic variables

- Macro. stress: F/A
- Macro. strain: δ/L



Compression test on a concrete sample
(Courtesy S. Bahafid, S. Ghabezloo)

Bottom-up (numerical) prediction

- The **corrector problem** reproduces physical experiment in-silico!
- The virtual sample is the so-called **representative volume element (RVE)**
- No body forces, loading through boundary conditions

Field equations

Boundary conditions

Must satisfy the Hill–Mandel condition

$$\nabla_x \cdot \boldsymbol{\sigma} = \mathbf{0}$$

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x})$$

$$\boldsymbol{\varepsilon} = \nabla^s \mathbf{u}$$

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

Example: homogeneous strain boundary conditions

$$\mathbf{u}(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x} \quad \Rightarrow \quad \langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}$$

Effective properties

Formal definition

From the linearity of the corrector problem

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

Macroscopic energy: from the Hill–Mandel condition

$$\frac{1}{2} \langle \boldsymbol{\varepsilon} : \mathbf{C} : \boldsymbol{\varepsilon} \rangle = \frac{1}{2} \langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle = \frac{1}{2} \langle \boldsymbol{\sigma} \rangle : \langle \boldsymbol{\varepsilon} \rangle = \frac{1}{2} (\mathbf{C}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle) : \langle \boldsymbol{\varepsilon} \rangle$$

To sum up

$$\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}} \quad \langle \boldsymbol{\sigma} \rangle = \mathbf{C}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle \quad \frac{1}{2} \langle \boldsymbol{\varepsilon} : \mathbf{C} : \boldsymbol{\varepsilon} \rangle = \frac{1}{2} \langle \boldsymbol{\varepsilon} \rangle : \mathbf{C}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle$$

The strain localization operator

The corrector problem is linear

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{A}(\mathbf{x}) : \bar{\boldsymbol{\varepsilon}}$$

Minor symmetries but not major symmetry!

Effective stiffness from macroscopic stress (symmetry?)

$$\mathbf{C}^{\text{eff}} : \bar{\boldsymbol{\varepsilon}} = \langle \boldsymbol{\sigma} \rangle = \langle \mathbf{C} : \mathbf{A} \rangle : \bar{\boldsymbol{\varepsilon}} \quad \Rightarrow \quad \mathbf{C}^{\text{eff}} = \langle \mathbf{C} : \mathbf{A} \rangle$$

Effective stiffness from macroscopic energy (symmetry!)

$$\bar{\boldsymbol{\varepsilon}} : \mathbf{C}^{\text{eff}} : \bar{\boldsymbol{\varepsilon}} = \langle \boldsymbol{\varepsilon} : \mathbf{C} : \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}} : \langle \mathbf{A}^T : \mathbf{C} : \mathbf{A} \rangle : \bar{\boldsymbol{\varepsilon}} \quad \Rightarrow \quad \mathbf{C}^{\text{eff}} = \langle \mathbf{A}^T : \mathbf{C} : \mathbf{A} \rangle$$

The case of eigenstrained materials

The corrector problem

$$\begin{aligned} \mathbf{x} \in \Omega : \quad & \begin{cases} \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} = \mathbf{0} \\ \boldsymbol{\sigma}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : [\boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\eta}(\mathbf{x})] \\ \boldsymbol{\varepsilon} = \nabla^S \mathbf{u} \end{cases} \\ \mathbf{x} \in \partial\Omega : \quad & \mathbf{u}(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}} \cdot \mathbf{x} \end{aligned}$$

Effective constitutive law (Levin, 1967 [1])

$$\begin{aligned} \langle \boldsymbol{\sigma} \rangle &= \mathbf{C}^{\text{eff}} : [\langle \boldsymbol{\varepsilon} \rangle - \boldsymbol{\eta}^{\text{eff}}] \\ \mathbf{C}^{\text{eff}} &= \langle \mathbf{C} : \mathbf{A} \rangle \quad \text{and} \quad \mathbf{C}^{\text{eff}} : \boldsymbol{\eta}^{\text{eff}} = \langle \mathbf{A}^T : \mathbf{C} : \boldsymbol{\eta} \rangle \end{aligned}$$

All you need is the localization operator!

[1] N. Laws, *Journal of the Mechanics and Physics of Solids* **1973**, 21, 9–17.

Note on the macroscopic energy

Microscopic volume density of energy

$$\frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\eta}) : \mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\eta})$$

Macroscopic volume density of energy

$$\begin{aligned} & \langle \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\eta}) : \mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\eta}) \rangle \\ &= \frac{1}{2}\langle \boldsymbol{\varepsilon} : \mathbf{C} : \boldsymbol{\varepsilon} \rangle - \langle \boldsymbol{\varepsilon} : \mathbf{C} : \boldsymbol{\eta} \rangle + \frac{1}{2}\langle \boldsymbol{\eta} : \mathbf{C} : \boldsymbol{\eta} \rangle \\ &= \frac{1}{2}\langle \bar{\boldsymbol{\varepsilon}} : \mathbf{A}^T : \mathbf{C} : \mathbf{A} : \bar{\boldsymbol{\varepsilon}} \rangle - \langle \bar{\boldsymbol{\varepsilon}} : \mathbf{A}^T : \mathbf{C} : \boldsymbol{\eta} \rangle + \frac{1}{2}\langle \boldsymbol{\eta} : \mathbf{C} : \boldsymbol{\eta} \rangle \\ &= \frac{1}{2}\bar{\boldsymbol{\varepsilon}} : \langle \mathbf{A}^T : \mathbf{C} : \mathbf{A} \rangle : \bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}} : \langle \mathbf{A}^T : \mathbf{C} : \boldsymbol{\eta} \rangle + \frac{1}{2}\langle \boldsymbol{\eta} : \mathbf{C} : \boldsymbol{\eta} \rangle \\ &= \frac{1}{2}\langle \boldsymbol{\varepsilon} \rangle : \mathbf{C}^{\text{eff}} : \langle \boldsymbol{\varepsilon} \rangle - \langle \boldsymbol{\varepsilon} \rangle : \mathbf{C}^{\text{eff}} : \boldsymbol{\eta}^{\text{eff}} + \frac{1}{2}\langle \boldsymbol{\eta} : \mathbf{C} : \boldsymbol{\eta} \rangle \\ &= \frac{1}{2}(\langle \boldsymbol{\varepsilon} \rangle - \boldsymbol{\eta}^{\text{eff}}) : \mathbf{C}^{\text{eff}} : (\langle \boldsymbol{\varepsilon} \rangle - \boldsymbol{\eta}^{\text{eff}}) + \underbrace{\frac{1}{2}\langle \boldsymbol{\eta} : \mathbf{C} : \boldsymbol{\eta} \rangle - \frac{1}{2}\langle \boldsymbol{\eta}^{\text{eff}} : \mathbf{C}^{\text{eff}} : \boldsymbol{\eta}^{\text{eff}} \rangle}_{\text{Constant}} \end{aligned}$$

On mean-field / effective-field models

N -phase materials: assumptions

- Properties are constant in each phase

$$\mathbf{x} \in \Omega_\alpha : \quad \mathbf{C}(\mathbf{x}) = \mathbf{C}_\alpha \quad \text{and} \quad \boldsymbol{\eta}(\mathbf{x}) = \boldsymbol{\eta}_\alpha \quad (\alpha = 1, \dots, N)$$

- Stresses and strains are approximated by constants in each phase

$$\mathbf{x} \in \Omega_\alpha : \quad \boldsymbol{\sigma}(\mathbf{x}) \simeq \boldsymbol{\sigma}_\alpha \quad \text{and} \quad \boldsymbol{\varepsilon}(\mathbf{x}) \simeq \boldsymbol{\varepsilon}_\alpha \quad (\alpha = 1, \dots, N)$$

- Localization tensors

$$\boldsymbol{\varepsilon}_\alpha = \mathbf{A}_\alpha : \bar{\boldsymbol{\varepsilon}} \quad \text{with} \quad f_1 \mathbf{A}_1 + \cdots + f_N \mathbf{A}_N = \mathbf{I}$$

Estimates of the effective properties

$$\mathbf{C}^{\text{eff}} \simeq f_1 \mathbf{C}_1 : \mathbf{A}_1 + \cdots + f_N \mathbf{C}_N : \mathbf{A}_N$$

$$\mathbf{C}^{\text{eff}} : \boldsymbol{\eta}^{\text{eff}} \simeq f_1 \mathbf{A}_1^\top : \mathbf{C}_1 : \boldsymbol{\eta}_1 + \cdots + f_N \mathbf{A}_N^\top : \mathbf{C}_N : \boldsymbol{\eta}_N$$

Eshelby's inhomogeneity problem [1]

Strain within ellipsoid is uniform

$$\boldsymbol{\varepsilon}_i = \mathbf{A}^\infty(\mathbf{C}_i, \mathbf{C}_m) : \boldsymbol{\varepsilon}^\infty$$

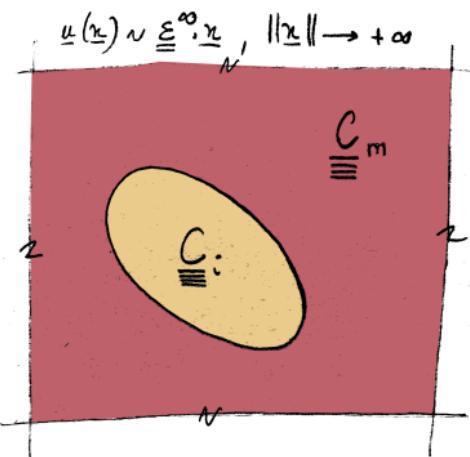
The dilute strain localization tensor

$$\mathbf{A}^\infty(\mathbf{C}_i, \mathbf{C}_m) = [\mathbf{I} + \mathbf{P}(\mathbf{C}_m) : (\mathbf{C}_i - \mathbf{C}_m)]^{-1}$$

Hill tensor of a sphere (isotropic mat)

$$\mathbf{P}(\mu, \nu) = \frac{1 - 2\nu}{6\mu(1 - \nu)} \mathbf{J} + \frac{4 - 5\nu}{15\mu(1 - \nu)} \mathbf{K}$$

$$\mathbf{J} = \frac{1}{3} \boldsymbol{\delta} \otimes \boldsymbol{\delta} \quad \mathbf{K} = \mathbf{I} - \mathbf{J}$$



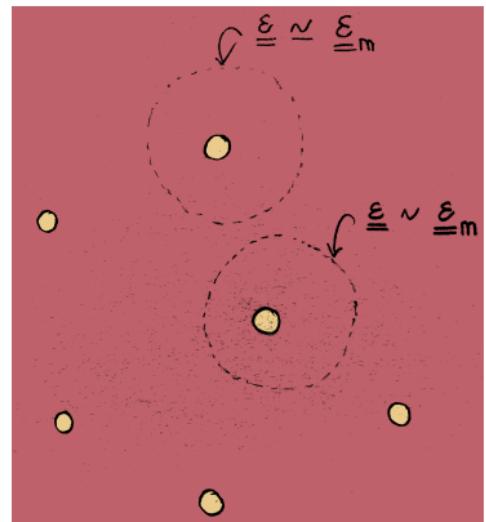
[1] J. D. Eshelby, *Proceedings of the Royal Society of London. Series A Mathematical and Physical Sciences* **1957**, 241, 376–396.

Mori–Tanaka estimate (explicit)

Each inclusion sees only the matrix

$$\begin{cases} \boldsymbol{\varepsilon}_i = \mathbf{A}^\infty(\mathbf{C}_i, \mathbf{C}_m) : \boldsymbol{\varepsilon}_m \\ \langle \boldsymbol{\varepsilon} \rangle = f_i \boldsymbol{\varepsilon}_i + f_m \boldsymbol{\varepsilon}_m \\ \langle \boldsymbol{\sigma} \rangle = f_i \mathbf{C}_i : \boldsymbol{\varepsilon}_i + f_m \mathbf{C}_m : \boldsymbol{\varepsilon}_m \end{cases}$$

$$\begin{cases} \mathbf{A}_m^{MT} = [f_i \mathbf{A}^\infty(\mathbf{C}_i, \mathbf{C}_m) + f_m \mathbf{I}]^{-1} \\ \mathbf{A}_i^{MT} = \mathbf{A}^\infty(\mathbf{C}_i, \mathbf{C}_m) : \mathbf{A}_m^{MT} \\ \mathbf{C}^{MT} = f_i \mathbf{C}_i : \mathbf{A}_i + f_m \mathbf{C}_m : \mathbf{A}_m \end{cases}$$



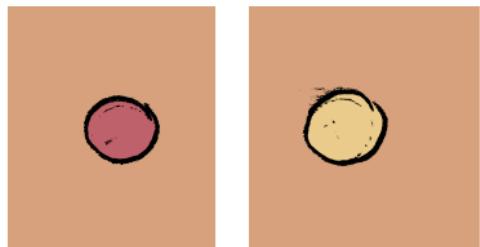
Self-consistent estimate (implicit)

Each phase sees the effective medium

$$\left\{ \begin{array}{l} \boldsymbol{\varepsilon}_0 = \mathbf{A}^\infty(\mathbf{C}_0, \mathbf{C}^{sc}) : \boldsymbol{\varepsilon}^\infty \\ \boldsymbol{\varepsilon}_1 = \mathbf{A}^\infty(\mathbf{C}_1, \mathbf{C}^{sc}) : \boldsymbol{\varepsilon}^\infty \\ \langle \boldsymbol{\varepsilon} \rangle = f_0 \boldsymbol{\varepsilon}_1 + f_1 \boldsymbol{\varepsilon}_m \\ \langle \boldsymbol{\sigma} \rangle = f_0 \mathbf{C}_0 : \boldsymbol{\varepsilon}_0 + f_1 \mathbf{C}_1 : \boldsymbol{\varepsilon}_1 \end{array} \right.$$



$$\left\{ \begin{array}{l} \mathbf{A}_\alpha^\infty = \mathbf{A}^\infty(\mathbf{C}_\alpha, \mathbf{C}^{sc}) \\ \mathbf{A}_\infty^{sc} = (f_0 \mathbf{A}_0^\infty + f_1 \mathbf{A}_1^\infty)^{-1} \\ \mathbf{A}_\alpha = \mathbf{A}_\alpha^\infty : \mathbf{A}_\infty^{sc} \\ \mathbf{C}^{sc} = f_0 \mathbf{C}_0 : \mathbf{A}_0 + f_1 \mathbf{C}_1 : \mathbf{A}_1 \end{array} \right.$$



Homogenization models in one slide

What is required

- Microstructure fully defined by volume fraction f_1 ($f_0 + f_1 = 1$)
- Homogenization model fully defined by localization tensor:

$$\mathbf{A}_1(f_1, \mathbf{C}_0, \mathbf{C}_1) \quad (f_0 \mathbf{A}_0 + f_1 \mathbf{A}_1 = \mathbf{I}).$$

Effective stiffness

$$\mathbf{C}^{\text{eff}} = f_0 \mathbf{C}_0 : \mathbf{A}_0 + f_1 \mathbf{C}_1 : \mathbf{A}_1$$

Effective eigenstrain

$$\mathbf{C}^{\text{eff}} : \boldsymbol{\eta}^{\text{eff}} = f_0 \mathbf{A}_0^\top : \mathbf{C}_0 : \boldsymbol{\eta}_0 + f_1 \mathbf{A}_1^\top : \mathbf{C}_1 : \boldsymbol{\eta}_1$$

Effective energy

$$\frac{1}{2} (\bar{\boldsymbol{\epsilon}} - \boldsymbol{\eta}^{\text{eff}}) : \mathbf{C}^{\text{eff}} : (\bar{\boldsymbol{\epsilon}} - \boldsymbol{\eta}^{\text{eff}})$$

Application to phase-field models

Volume fractions

Most simple form

$$\begin{aligned}\phi = 0 &\rightarrow \text{phase 0 only} \\ \phi = 1 &\rightarrow \text{phase 1 only}\end{aligned}\Rightarrow \phi = \text{volume fraction of phase 1?}$$

More flexible form

$$h(\phi) = \text{volume fraction of phase 1}$$

$$\bar{h}(\phi) = 1 - h(\phi) = \text{volume fraction of phase 0}$$

with the conditions

$$h(0) = 0 \quad h(1) = 1 \quad h'(0) = 0 \quad h'(1) = 1$$

Free energy (mechanical contribution)

The homogenization model

$$\mathbf{A}_1(f_1, \mathbf{C}_0, \mathbf{C}_1) \quad \text{with} \quad f_1 = h(\phi) \quad \text{and} \quad \mathbf{C}_0, \mathbf{C}_1 \quad \text{fixed} \quad \Rightarrow \quad \mathbf{A}_1[h(\phi)]$$

Homogenized energy

$$f_\varepsilon(\phi, \boldsymbol{\varepsilon}) = \frac{1}{2} (\boldsymbol{\varepsilon} - \boldsymbol{\eta}) : \mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\eta})$$

with

$$\mathbf{C} = \bar{h} \mathbf{C}_0 : \mathbf{A}_0 + h \mathbf{C}_1 : \mathbf{A}_1$$

and

$$\mathbf{C} : \boldsymbol{\eta} = \bar{h} \mathbf{A}_0^\top : \mathbf{C}_0 : \boldsymbol{\eta}_0 + h \mathbf{A}_1^\top : \mathbf{C}_1 : \boldsymbol{\eta}_1$$

Notes on practical implementation

- Constitutive laws require first derivatives of f_ε w.r.t. ϕ and $\boldsymbol{\varepsilon}$
- Newton iterations require higher order derivatives
- Derivatives w.r.t. volume fraction $h(\phi)$ can be quite painful for some homogenization models (e.g. self-consistent)
- Tabulate values for $0 \leq h(\phi) \leq 1$
- Use implicit function theorem?
- Use automatic differentiation?

Applications

Linear interpolation

$$\mathbf{C} = \bar{h}\mathbf{C}_0 + h\mathbf{C}_1$$

$$\boldsymbol{\eta} = \bar{h}\boldsymbol{\eta}_0 + h\boldsymbol{\eta}_1$$

Voigt approximation

$$\mathbf{A}_0 = \mathbf{A}_1 = \mathbf{I} \quad \Rightarrow \quad \begin{cases} \mathbf{C} = \bar{h}\mathbf{C}_0 + h\mathbf{C}_1 \\ \mathbf{C} : \boldsymbol{\eta} = \bar{h}\mathbf{C}_0 : \boldsymbol{\eta}_0 + h\mathbf{C}_1 : \boldsymbol{\eta}_1 \end{cases}$$

Reuss approximation

$$\mathbf{C}_0 : \mathbf{A}_0 = \mathbf{C}_1 : \mathbf{A}_1 = \mathbf{C} \quad \Rightarrow \quad \begin{cases} \mathbf{C}^{-1} = \bar{h}\mathbf{C}_0^{-1} + h\mathbf{C}_1^{-1} \\ \boldsymbol{\eta} = \bar{h}\boldsymbol{\eta}_0 + h\boldsymbol{\eta}_1 \end{cases}$$

Extensions

- Extension to diffusion? (homogenized mobility?)
- Laminate theory

$$\mathbf{C}^{\text{eff}}(f_1, \mathbf{C}_0, \mathbf{C}_1, \mathbf{n}) \quad \text{with} \quad f_1 = h(\phi) \quad \text{and} \quad \mathbf{n} = \frac{\nabla\phi}{\|\nabla\phi\|}$$

- Material non-linearities
- Geometric non-linearities

Thank you for your attention!

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<https://cv.archives-ouvertes.fr/sbrisard>

<https://sbrisard.github.io>



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