Nonlinear homogenization

(from 1983 to present days and beyond)

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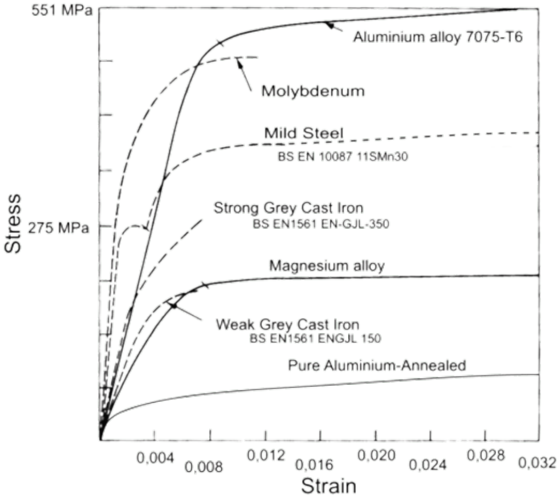
Whence the nonlinearity?



$$\boldsymbol{\sigma} = F(\boldsymbol{\varepsilon}) \neq \mathbb{C}\boldsymbol{\varepsilon}$$

Whence the nonlinearity?

- How does plastic strength of a composite vary with fiber content?
- How does viscoplastic flow of a polycrystalline solid vary with the evolving microstructure?
- How does viscoelasticity of a soft solid vary with reinforcement content?
- Other nonlinear behavioral aspects: ferroelectricity, ferromagnetism, dielectric strength, loss of superconductivity, etc.

Convex nonlinearity

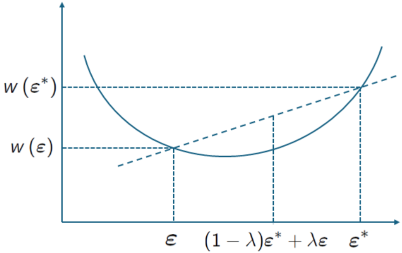
We will consider stress-strain relations of the form

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \varepsilon}(\varepsilon)$$

where $w(\cdot)$ is strictly convex and bounded from below, i.e.,

$$w\left((1-\lambda)\varepsilon^* + \lambda\varepsilon\right) < (1-\lambda)w\left(\varepsilon^*\right) + \lambda w\left(\varepsilon\right)$$

for all $0 < \lambda < 1$ and $\varepsilon \neq \varepsilon^*$.



Convex nonlinearity

Inverse stress-strain relation

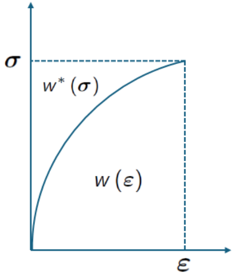
$$\varepsilon = \frac{\partial w^*}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma})$$

where the complementary energy $w^*(\cdot)$ is the Legendre transform of $w(\cdot)$ defined as

$$w^*(\boldsymbol{\sigma}) = \sup_{\boldsymbol{\varepsilon}} [\boldsymbol{\sigma} \cdot \varepsilon - w(\varepsilon)] .$$

The function $w^*(\cdot)$ is strictly convex.
Taking the Legendre transform of $w^*(\cdot)$ yields the original function

$$w(\varepsilon) = w^{**}(\varepsilon) = \sup_{\boldsymbol{\sigma}} [\boldsymbol{\sigma} \cdot \varepsilon - w^*(\boldsymbol{\sigma})] .$$



Convex nonlinearity: power-law relations

For instance, uniaxial power-law relations

$$\frac{\sigma_e}{\sigma_0} = \left(\frac{\varepsilon_e}{\varepsilon_0}\right)^m$$

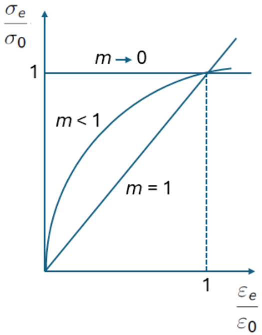
with $0 < m \leq 1$, correspond to incompressible tensorial relations of the form

$$\boldsymbol{\sigma} = \frac{2}{3}\sigma_0 \left(\frac{\varepsilon_e}{\varepsilon_0}\right)^m \frac{\boldsymbol{\varepsilon}_d}{\varepsilon_e} - p\,\mathsf{I}, \quad \boldsymbol{\varepsilon} = \frac{3}{2}\varepsilon_0 \left(\frac{\sigma_e}{\sigma_0}\right)^m \frac{\boldsymbol{\sigma}_d}{\sigma_e}$$

and energies of the form

$$w(\boldsymbol{\varepsilon}) = \frac{\sigma_0\varepsilon_0}{1+m}\left(\frac{\varepsilon_e}{\varepsilon_0}\right)^{1+m} - \sup_p p\,\mathrm{tr}\boldsymbol{\varepsilon}$$

$$w^*(\boldsymbol{\sigma}) = \frac{\sigma_0\varepsilon_0}{1+n}\left(\frac{\sigma_e}{\sigma_0}\right)^{1+n}, \quad n = 1/m \geq 1$$



Von Mises equivalent strain and stress:

$$\varepsilon_e = \sqrt{\frac{2}{3}\boldsymbol{\varepsilon}_d \cdot \boldsymbol{\varepsilon}_d} \quad \sigma_e = \sqrt{\frac{3}{2}\boldsymbol{\sigma}_d \cdot \boldsymbol{\sigma}_d}$$

Outline

1. The homogenized response $\rightarrow$ effective energy
2. Elementary bounds on the effective energy
3. Linear-comparison bounds on the effective energy
4. Weak-contrast expansion of the effective energy
5. Linear-comparison estimates of the effective energy

The homogenized response: effective energy

- Homogenized or effective response

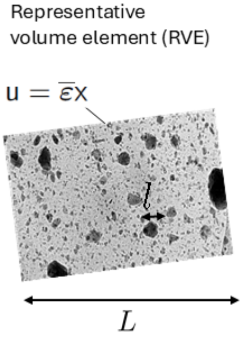
$$\overline{\boldsymbol{\sigma}} = \frac{\partial \overline{w}}{\partial \overline{\boldsymbol{\varepsilon}}}(\overline{\boldsymbol{\varepsilon}})$$

where

$$\overline{\boldsymbol{\varepsilon}} = \langle \boldsymbol{\varepsilon}(\mathrm{x}) \rangle \quad \overline{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma}(\mathrm{x}) \rangle \quad \overline{w}(\overline{\boldsymbol{\varepsilon}}) = \langle w(\mathrm{x}, \boldsymbol{\varepsilon}(\mathrm{x})) \rangle$$

- Field equations within RVE (in the sense of distributions)

$$\begin{aligned} \text{equilibrium:} \quad & 0 = \nabla \cdot \boldsymbol{\sigma} \\ \text{compatibility:} \quad & \boldsymbol{\varepsilon} = \nabla \otimes_s \mathrm{u} \\ \text{const. rel.:} \quad & \boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\mathrm{x}, \boldsymbol{\varepsilon}) \\ \text{boundary cond.:} \quad & \mathrm{u} = \overline{\boldsymbol{\varepsilon}}\mathrm{x} \text{ or } \mathrm{t} = \overline{\boldsymbol{\sigma}}\mathrm{n} \end{aligned}$$



$$\frac{l}{L} \ll 1$$

Marcellini (1978), Willis (1989), Braides and Defranceschi (1998)

The homogenized response: effective energy

- Homogenized or effective response

$$\overline{\boldsymbol{\sigma}} = \frac{\partial \overline{w}}{\partial \overline{\varepsilon}}(\overline{\varepsilon})$$

  where the effective energy is

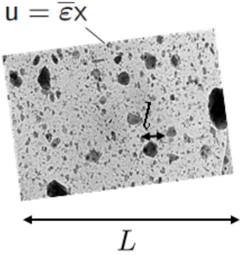
$$\overline{w}(\overline{\varepsilon}) = \min_{\varepsilon \in \mathcal{K}(\overline{\varepsilon})} \langle w\,(\mathrm{x}, \varepsilon)\rangle$$

  over the set of kinematically admissible strain fields

$$\mathcal{K}(\overline{\varepsilon}) = \{\varepsilon(\mathrm{x}) \text{ such that } \varepsilon = \nabla \otimes_s \mathrm{u} \text{ in } \Omega \\ \text{and } \mathrm{u} = \overline{\varepsilon}\mathrm{x} \text{ on } \partial\Omega\}$$

- The effective energy $\overline{w}$ inherits the convexity of the local energy w

Representative
volume element (RVE)



$$\frac{l}{L} \ll 1$$

Marcellini (1978), Willis (1989), Braides and Defranceschi (1998)

The homogenized response: complementary effective energy

- Inverse effective response

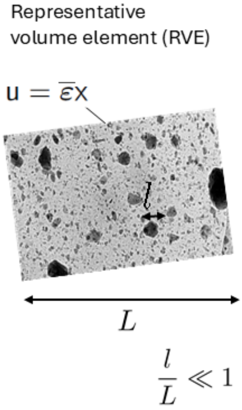
$$\overline{\boldsymbol{\varepsilon}} = \frac{\partial \overline{w}^*}{\partial \overline{\boldsymbol{\sigma}}}(\overline{\boldsymbol{\sigma}})$$

where the complementary effective energy is

$$\overline{w}^*(\overline{\boldsymbol{\sigma}}) = \min_{\boldsymbol{\sigma} \in \mathcal{S}(\overline{\boldsymbol{\sigma}})} \langle w^*(\mathrm{x}, \boldsymbol{\sigma}) \rangle$$

over the set of statically admissible stress fields

$$\mathcal{S}(\overline{\boldsymbol{\sigma}}) = \{\boldsymbol{\sigma}(\mathrm{x}) \text{ such that } \nabla \cdot \boldsymbol{\sigma} = 0 \text{ in } \Omega \\ \text{and } \boldsymbol{\sigma}\mathrm{n} = \overline{\boldsymbol{\sigma}}\mathrm{n} \text{ on } \partial\Omega\}$$



Willis (1989)

The homogenized response: power-law relations

For phase energies of the form

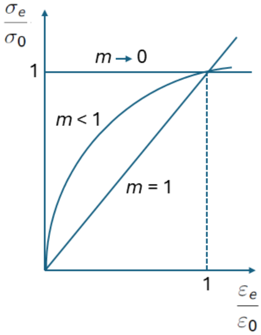
$$w^{(r)}(\varepsilon) = \frac{\sigma_0^{(r)}\varepsilon_0}{1+m}\left(\frac{\varepsilon_e}{\varepsilon_0}\right)^{1+m} - \sup_p p \operatorname{tr}\varepsilon$$

the effective energy is of the form

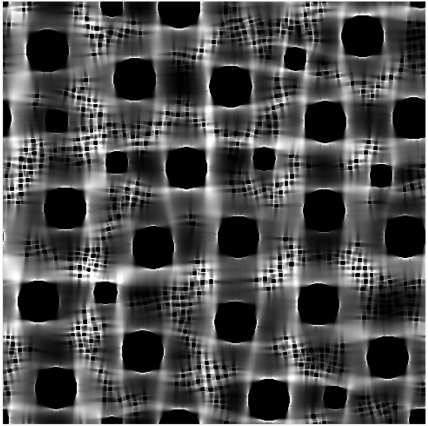
$$\overline{w}(\overline{\varepsilon}) = \min_{\varepsilon \in \mathcal{K}_i(\overline{\varepsilon})} \sum_{r=1}^{N} c^{(r)} \left\langle \frac{\sigma_0^{(r)}\varepsilon_0}{1+m}\left(\frac{\varepsilon_e}{\varepsilon_0}\right)^{1+m} \right\rangle^{(r)}$$

$$= \min_{\varepsilon' \in \mathcal{K}_i(\overline{\varepsilon}/\overline{\varepsilon}_e)} \sum_{r=1}^{N} c^{(r)} \left\langle \sigma_0^{(r)} {\varepsilon'_e}^{1+m} \right\rangle^{(r)} \frac{\varepsilon_0}{1+m}\left(\frac{\overline{\varepsilon}_e}{\varepsilon_0}\right)^{1+m}$$

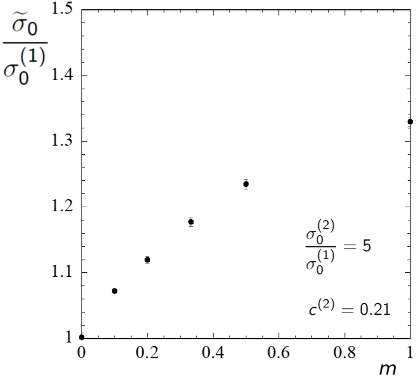
$$= \frac{\widetilde{\sigma}_0(\dots)\varepsilon_0}{1+m}\left(\frac{\overline{\varepsilon}_e}{\varepsilon_0}\right)^{1+m} \qquad \widetilde{\sigma}_0(\dots) = \widetilde{\sigma}_0(\overline{\varepsilon}/\overline{\varepsilon}_e, m, \sigma^{(r)})$$



Convex nonlinearity: power-law relations



strain distribution in a fiber-reinforced composite under simple shear when $m = 0.1$



Idiart, Moulinec, Ponte Castañeda and Suquet (2006)

Outline

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Elementary upper bound

- Evaluate the average energy at $\varepsilon(\mathrm{x}) = \overline{\varepsilon}$ in $\mathcal{K}(\overline{\varepsilon})$:

$$\overline{w}(\overline{\varepsilon}) \leq \overline{w}_{+}(\overline{\varepsilon}) = \langle w(\mathrm{x}, \overline{\varepsilon}) \rangle = \sum_{r=1}^{N} c^{(r)} \langle w^{(r)}(\overline{\varepsilon}) \rangle^{(r)} = \sum_{r=1}^{N} c^{(r)} w^{(r)}(\overline{\varepsilon})$$

- This upper bound amounts to a "nonlinear" rule of mixtures. It is referred to as the "Voigt" bound
- The Voigt bound is convex
- The Voigt bound can be used to generate the approximate stress-strain relation

$$\overline{\boldsymbol{\sigma}} = \frac{\partial \overline{w}_{+}}{\partial \overline{\varepsilon}}(\overline{\varepsilon}) = \sum_{r=1}^{N} c^{(r)} \frac{\partial w^{(r)}}{\partial \varepsilon}(\overline{\varepsilon})$$

Voigt (1889), Hill (1952)

Elementary lower bound

- Write the effective energy as

$$\overline{w}(\overline{\varepsilon}) = \min_{\varepsilon \in \mathcal{K}(\overline{\varepsilon})} \sup_{\boldsymbol{\sigma}} \langle \boldsymbol{\sigma} \cdot \varepsilon - w^*(\mathrm{x}, \boldsymbol{\sigma}) \rangle$$

- Evaluate the average energy at $\boldsymbol{\sigma}(\mathrm{x}) = \overline{\boldsymbol{\sigma}}$:

$$\overline{w}(\overline{\varepsilon}) \geq \overline{w}_-(\overline{\varepsilon}) = \min_{\varepsilon \in \mathcal{K}(\overline{\varepsilon})} \sup_{\boldsymbol{\sigma}} \langle \overline{\boldsymbol{\sigma}} \cdot \varepsilon - w^*(\mathrm{x}, \overline{\boldsymbol{\sigma}}) \rangle = \sup_{\overline{\boldsymbol{\sigma}}} \left[\overline{\boldsymbol{\sigma}} \cdot \overline{\varepsilon} - \sum_{r=1}^{N} c^{(r)} w^{(r)^*}(\overline{\boldsymbol{\sigma}}) \right]$$

$$= \sup_{\overline{\boldsymbol{\sigma}}} \left[\overline{\boldsymbol{\sigma}} \cdot \overline{\varepsilon} - \overline{w}_-^*(\overline{\boldsymbol{\sigma}}) \right] = \overline{w}_-(\overline{\varepsilon})$$

- This lower bound is referred to as the "Reuss" bound, which is convex
- The Reuss bound can be used to generate the approximate stress-strain relation

$$\overline{\varepsilon} = \frac{\partial \overline{w}_-^*}{\partial \overline{\boldsymbol{\sigma}}}(\overline{\boldsymbol{\sigma}}) = \sum_{r=1}^{N} c^{(r)} \frac{\partial w^{(r)^*}}{\partial \boldsymbol{\sigma}}(\overline{\boldsymbol{\sigma}})$$

Reuss (1929), Hill (1952)

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Elementary bounds for power-law composites

For phase energies of the form

$$w^{(r)}(\boldsymbol{\varepsilon}) = \frac{\sigma_0^{(r)}\varepsilon_0}{1+m}\left(\frac{\varepsilon_e}{\varepsilon_0}\right)^{1+m} - \sup_p p\,\mathrm{tr}\boldsymbol{\varepsilon}$$

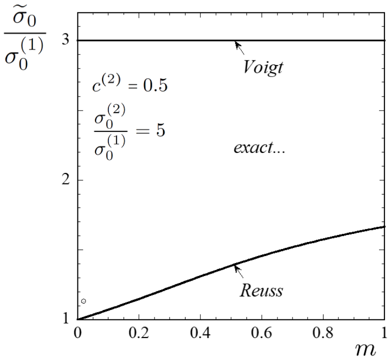
the bounds are of the form

$$\overline{w}_+(\overline{\boldsymbol{\varepsilon}}) = \frac{\widetilde{\sigma}_+\varepsilon_0}{1+m}\left(\frac{\overline{\varepsilon}_e}{\varepsilon_0}\right)^{1+m} - \sup_p p\,\mathrm{tr}\overline{\boldsymbol{\varepsilon}}$$

$$\overline{w}_-(\overline{\boldsymbol{\varepsilon}}) = \frac{\widetilde{\sigma}_-\varepsilon_0}{1+m}\left(\frac{\overline{\varepsilon}_e}{\varepsilon_0}\right)^{1+m} - \sup_p p\,\mathrm{tr}\overline{\boldsymbol{\varepsilon}}$$

where

$$\left(\sum_{r=1}^{N} c^{(r)}\sigma_0^{(r)\,-m}\right)^{-1/m} = \widetilde{\sigma}_- \leq \widetilde{\sigma}_0(\overline{\boldsymbol{\varepsilon}}/\overline{\varepsilon}_e) \leq \widetilde{\sigma}_+ = \sum_{r=1}^{N} c^{(r)}\sigma_0^{(r)}$$



Elementary bounds

- Voigt and Reuss bounds agree to first order in the heterogeneity contrast $\Rightarrow$ exact in that case
- However, they diverge as heterogeneity contrast increases
- They provide very poor predictions for strong contrasts
- They depend on first-order microstructural information (volume fractions) only
- Prehistoric efforts to incorporate microstructural morphology into predictions:
    - Hill (1965): incremental method
    - Hutchinson (1970,1976,1977)
    - Dvorak and Bahei-En-Din (1979)
    - Berveiller and Zaoui (1979): secant method

among others that followed...

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Linear-comparison bounds

Some efforts to develop bounds that account for microstructural morphology:

- Willis (1983,1984,1986,1989,1992,1994), Talbot and Willis (1985,1986,1987,1991), Ponte Castañeda and Willis (1988), Toland and Willis (1989), Dendievel et al. (1990)
- Ponte Castañeda (1991,1992)
- Suquet (1992,1993,1995,1996,1997)
- Ponte Castañeda and Willis (1992), Ponte Castañeda and Suquet (1998)
- Idiart and Ponte Castañeda (2007), Idiart (2012)

Central idea:

exploit convex inequalities to identify 'optimal' linearizations that allow the use of linear bounds that account for microstructural morphology to generate corresponding non-linear bounds, hence the terminology 'linear-comparison bounds'.

Linear-comparison bounds

For a given a sub-quadratic even phase potential $w^{(r)}(\varepsilon)$, let

$$v^{(r)}\left(\mathbb{C}^{(r)}\right) = \sup_{\varepsilon}\left\{w^{(r)}(\varepsilon) - \frac{1}{2}\varepsilon\cdot\mathbb{C}^{(r)}\varepsilon\right\}$$

be a function of positive-definite 'elasticity' tensors $\mathbb{C}^{(r)}$. By definition,

$$v^{(r)}\left(\mathbb{C}^{(r)}\right) \geq w^{(r)}(\varepsilon) - \frac{1}{2}\varepsilon\cdot\mathbb{C}^{(r)}\varepsilon \quad \Rightarrow \quad w^{(r)}(\varepsilon) \leq \frac{1}{2}\varepsilon\cdot\mathbb{C}^{(r)}\varepsilon + v^{(r)}\left(\mathbb{C}^{(r)}\right)$$

Immediately, we obtain the upper bound on the effective energy

$$\overline{w}(\overline{\varepsilon}) = \min_{\varepsilon\,\in\,\mathcal{K}(\overline{\varepsilon})} \sum_{r=1}^{N} c^{(r)}\left\langle w^{(r)}(\varepsilon)\right\rangle^{(r)} \leq \min_{\varepsilon\,\in\,\mathcal{K}(\overline{\varepsilon})} \sum_{r=1}^{N} c^{(r)}\left\langle \frac{1}{2}\varepsilon\cdot\mathbb{C}^{(r)}\varepsilon + v^{(r)}\left(\mathbb{C}^{(r)}\right)\right\rangle^{(r)}$$

for *any* choice of 'elasticity' tensors $\mathbb{C}^{(r)}$.

Linear-comparison bounds

The 'best' upper bound is

$$\overline{w}(\overline{\varepsilon}) \leq \inf_{\mathbb{C}^{(r)} \geq 0} \left\{ \min_{\varepsilon \in \mathcal{K}(\overline{\varepsilon})} \sum_{r=1}^{N} c^{(r)} \left\langle \frac{1}{2} \varepsilon \cdot \mathbb{C}^{(r)} \varepsilon \right\rangle^{(r)} + v^{(r)} \left(\mathbb{C}^{(r)} \right) \right\}$$

Write this inequality as

$$\overline{w}(\overline{\varepsilon}) \leq \overline{w}_{+}(\overline{\varepsilon}) = \inf_{\mathbb{C}^{(r)} \geq 0} \left\{ \overline{w}_c(\overline{\varepsilon}; \mathbb{C}^{(r)}) + v^{(r)} \left(\mathbb{C}^{(r)} \right) \right\}$$

where

$$\Rightarrow \quad \overline{\boldsymbol{\sigma}} = \frac{\partial \overline{w}_{+}}{\partial \overline{\varepsilon}}(\overline{\varepsilon}) = \frac{\partial \overline{w}_c}{\partial \overline{\varepsilon}}(\overline{\varepsilon}; \mathbb{C}^{(r)}) = \widetilde{\mathbb{C}} \left(\mathbb{C}^{(r)}(\overline{\varepsilon}) \right) \overline{\varepsilon}$$

$$\overline{w}_c(\overline{\varepsilon}; \mathbb{C}^{(r)}) = \min_{\varepsilon \in \mathcal{K}(\overline{\varepsilon})} \sum_{r=1}^{N} c^{(r)} \left\langle \frac{1}{2} \varepsilon \cdot \mathbb{C}^{(r)} \varepsilon \right\rangle^{(r)} = \frac{1}{2} \overline{\varepsilon} \cdot \widetilde{\mathbb{C}} \overline{\varepsilon}$$

is the effective energy of a *linear-comparison composite* with the same microstructural morphology as the non-linear composite and with elastic phases characterized by 'optimal' elasticity tensors $\mathbb{C}^{(r)}$; $\overline{w}_{+}$ is convex.

This inequality can be used to generate non-linear upper bounds from linear upper bounds or exact results; it can also be used to generate non-linear estimates (rather than bounds) from linear estimates.

Linear-comparison bounds for power-law composites

For composites with isotropic microstructures and phase energies of the form

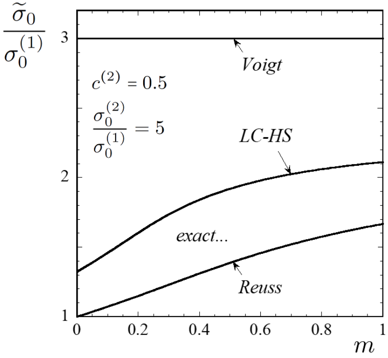
$$w^{(r)}(\varepsilon) = \frac{\sigma_0^{(r)}\varepsilon_0}{1+m}\left(\frac{\varepsilon_e}{\varepsilon_0}\right)^{1+m} - \sup_p p \, \mathrm{tr}\boldsymbol{\varepsilon}$$

the upper bound of the Hashin-Shtrikman type is of the form

$$\overline{w}_+(\overline{\varepsilon}) = \frac{\widetilde{\sigma}_+\varepsilon_0}{1+m}\left(\frac{\overline{\varepsilon}_e}{\varepsilon_0}\right)^{1+m} - \sup_p p \, \mathrm{tr}\overline{\boldsymbol{\varepsilon}}$$

with

$$\widetilde{\sigma}_+ = f(\sigma_0^{(r)}, c^{(r)}, m)$$



Ponte Castañeda (1991,1992)

Linear-comparison bounds

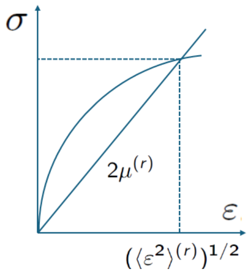
For isotropic incompressible phase energies of the form

$$w^{(r)}(\boldsymbol{\varepsilon}) = \phi^{(r)}(\varepsilon_e) - \sup_p p \,\mathrm{tr}\boldsymbol{\varepsilon}$$

the optimal $\mathbb{C}^{(r)}$ are isotropic incompressible tensors of the form (Suquet, 1995)

$$\mathbb{C}^{(r)} = +\infty\mathbb{J} + 2\mu^{(r)}\mathbb{K} \quad \text{with} \quad 3\mu^{(r)}\overline{\overline{\varepsilon}}_e^{(r)} = \phi^{(r)\prime}\left(\overline{\overline{\varepsilon}}_e^{(r)}\right)$$

which corresponds to a *secant linearization evaluated at the second moments* $\overline{\overline{\varepsilon}}_e^{(r)} = (\langle\varepsilon_e^2\rangle^{(r)})^{1/2}$ as opposed to earlier secant linearizations evaluated at the *first moments* (Berveiller and Zaoui, 1979), and the bound is



$$\overline{w}_+(\overline{\boldsymbol{\varepsilon}}) = \sum_{r=1}^{N} c^{(r)}\phi^{(r)}\left(\overline{\overline{\varepsilon}}_e^{(r)}\right)$$

Anisotropic phase energies require special results of convex analysis (Dendievel et al., 1990; deBotton and Ponte Castañeda, 1992; Ponte Castañeda and Suquet, 1998; Idiart and Ponte Castañeda, 2007, Idiart, 2012)

Linear-comparison bounds

Bounds on the (supra-quadratic) stress potential can also be derived by defining the functions

$$v^{(r)}\left(\mathbb{M}^{(r)}\right) = \inf_{\boldsymbol{\sigma}}\left\{w^{*(r)}(\boldsymbol{\sigma}) - \frac{1}{2}\boldsymbol{\sigma}\cdot\mathbb{M}^{(r)}\boldsymbol{\sigma}\right\}$$

of positive-definite 'compliance' tensors $\mathbb{M}^{(r)}$, so that

$$\overline{w}^*(\overline{\boldsymbol{\sigma}}) \geq \overline{w}^*_-(\overline{\boldsymbol{\sigma}}) = \sup_{\mathbb{M}^{(r)}\geq 0}\left\{\overline{w}^*_c(\overline{\boldsymbol{\sigma}};\mathbb{M}^{(r)}) + v^{(r)}\left(\mathbb{M}^{(r)}\right)\right\}$$

where

$$\overline{w}^*_c(\overline{\boldsymbol{\sigma}};\mathbb{M}^{(r)}) = \min_{\boldsymbol{\sigma}\,\in\,\mathcal{S}(\overline{\boldsymbol{\sigma}})}\sum_{r=1}^{N} c^{(r)}\left\langle\frac{1}{2}\boldsymbol{\sigma}\cdot\mathbb{M}^{(r)}\boldsymbol{\sigma}\right\rangle^{(r)} = \frac{1}{2}\overline{\boldsymbol{\sigma}}\cdot\widetilde{\mathbb{M}}\overline{\boldsymbol{\sigma}}$$

It is easy to show that

$$\overline{w}^{**}_-(\overline{\boldsymbol{\varepsilon}}) = \overline{w}_+(\overline{\boldsymbol{\varepsilon}}) \quad\Rightarrow\quad \text{we can only get one bound}$$

The strategy must be modified to develop the 'other' bound (Talbot and Willis, 1994).

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Weak-contrast expansion

Consider a local energy of the form

$$w(\mathrm{x}, \varepsilon) = w_0(\varepsilon) + t\ \delta w(\mathrm{x}, \varepsilon)$$

where t is small. The Taylor expansion of the effective energy to second order in t is (Suquet and Ponte Castañeda, 1993)

$$\overline{w}(\overline{\varepsilon}) = w_0(\overline{\varepsilon}) + t \sum_{r=1}^{N} c^{(r)} \delta w^{(r)}(\overline{\varepsilon}) - \frac{t^2}{2} \sum_{r=1}^{N} \sum_{s=1}^{N} \frac{\partial \delta w^{(r)}}{\partial \varepsilon}(\overline{\varepsilon}) \cdot \mathbb{G}^{(rs)}(\overline{\varepsilon}) \frac{\partial \delta w^{(s)}}{\partial \varepsilon}(\overline{\varepsilon}) + O(t^3)$$

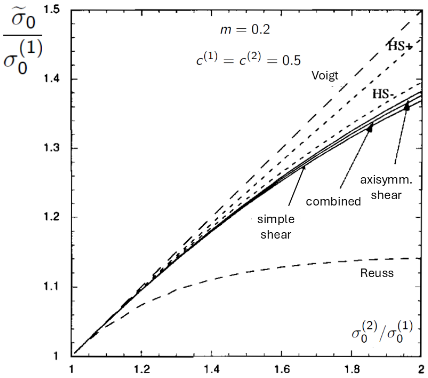
where the tensors $\mathbb{G}^{(rs)}(\overline{\varepsilon})$ depend on the two-point microstructural correlation functions $p^{(rs)}(\mathrm{x}, \mathrm{x}')$ and on the *tangent* tensor

$$\mathbb{C}^{(0)}(\overline{\varepsilon}) = \frac{\partial^2 w^{(0)}}{\partial \varepsilon \partial \varepsilon}(\overline{\varepsilon})$$

The expansion can break down for non-strictly convex energies (ideal plasticity).

Weak-contrast expansion: power-law composites

Isotropic incompressible composites
(Suquet and Ponte Castañeda, 1993)



- The elementary bounds and the linear-comparison bound of the Hashin-Shtrikman are exact to *first order in t only*
- The development of non-linear bounds that are exact to second order in t remains an open problem
- Can we at least develop non-linear estimates (rather than bounds) that are exact to second order in t?

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Tangent second-order estimates

For a given a sub-quadratic phase potential $w^{(r)}(\varepsilon)$, we could have defined the 'richer' function

$$v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right) = \sup_{\boldsymbol{\varepsilon}} \left\{ w^{(r)}(\boldsymbol{\varepsilon}) - \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} - \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} \right\}$$

so that, by definition,

$$v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right) \geq w^{(r)}(\boldsymbol{\varepsilon}) - \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} - \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} \quad \Rightarrow \quad w^{(r)}(\boldsymbol{\varepsilon}) \leq \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} + \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} + v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right)$$

and therefore

$$\overline{w}(\overline{\boldsymbol{\varepsilon}}) = \min_{\boldsymbol{\varepsilon}\,\in\,\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \sum_{r=1}^{N} c^{(r)} \left\langle w^{(r)}(\boldsymbol{\varepsilon}) \right\rangle^{(r)} \leq \inf_{\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}} \left\{ \min_{\boldsymbol{\varepsilon}\,\in\,\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \sum_{r=1}^{N} c^{(r)} \left\langle \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} + \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} + v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right) \right\rangle^{(r)} \right\}$$

Unfortunately, when the phase potentials $w^{(r)}(\boldsymbol{\varepsilon})$ are even the optimal polarizations are $\boldsymbol{\tau}^{(r)} = 0$ (Willis, 1992).

Tangent second-order estimates

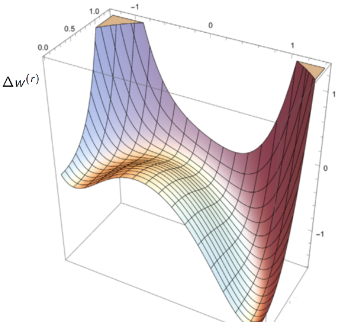
Motivated by this observation, Ponte Castañeda and Willis (1999) proposed the use of the alternative function

$$v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right) = \underset{\boldsymbol{\varepsilon}}{\text{stat}}\left\{w^{(r)}(\boldsymbol{\varepsilon}) - \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} - \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon}\right\}$$

which produces the alternative representation

$$w^{(r)}(\boldsymbol{\varepsilon}) = \underset{\boldsymbol{\tau}^{(r)}}{\text{stat}}\left\{\frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} + \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} + v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right)\right\}$$

and therefore the estimate



$$\overline{w}(\overline{\boldsymbol{\varepsilon}}) = \min_{\boldsymbol{\varepsilon}\,\in\,\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \sum_{r=1}^{N} c^{(r)}\left\langle w^{(r)}(\boldsymbol{\varepsilon})\right\rangle^{(r)} \approx \underset{\boldsymbol{\tau}^{(r)}}{\text{stat}}\left\{\min_{\boldsymbol{\varepsilon}\,\in\,\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \sum_{r=1}^{N} c^{(r)}\left\langle \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} + \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} + v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right)\right\rangle^{(r)}\right\}$$

Tangent second-order estimates

- The estimate is also based on the concept of a linear-comparison composite, but with a 'thermo-elastic' effective energy

$$\overline{w}_c(\overline{\boldsymbol{\varepsilon}};\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}) = \min_{\boldsymbol{\varepsilon}\,\in\,\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \sum_{r=1}^{N} c^{(r)} \left\langle \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} + \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} \right\rangle^{(r)} = \frac{1}{2}\overline{\boldsymbol{\varepsilon}}\cdot\widetilde{\mathbb{C}}\overline{\boldsymbol{\varepsilon}} + \widetilde{\boldsymbol{\tau}}\cdot\overline{\boldsymbol{\varepsilon}} + \widetilde{f}$$

- The functions $v^{(r)}$ are multivalued (there are *multiple* stationary points); the selection of suitable points is facilitated by the change of variables

$$\boldsymbol{\tau}^{(r)} = \frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}}(\breve{\boldsymbol{\varepsilon}}^{(r)}) - \mathbb{C}^{(r)}\breve{\boldsymbol{\varepsilon}}^{(r)}$$

so that stationarity with respect to $\boldsymbol{\tau}^{(r)}$ is replaced by the stationarity with respect to $\breve{\boldsymbol{\varepsilon}}^{(r)}$, which requires that

$$\breve{\boldsymbol{\varepsilon}}^{(r)} = \langle\boldsymbol{\varepsilon}\rangle^{(r)}$$

- The elasticity tensors $\mathbb{C}^{(r)}$ remain unspecified. Motivated by the second order expansion, Ponte Castañeda and Willis (1999) chose the tangent tensors

$$\mathbb{C}^{(r)} = \frac{\partial^2 w^{(r)}}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\varepsilon}}(\breve{\boldsymbol{\varepsilon}}^{(r)}) = \frac{\partial^2 w^{(r)}}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\varepsilon}}(\langle\boldsymbol{\varepsilon}\rangle^{(r)})$$

Tangent second-order estimates

- The final expression for the estimate can be written as (Ponte Castañeda, 1996)

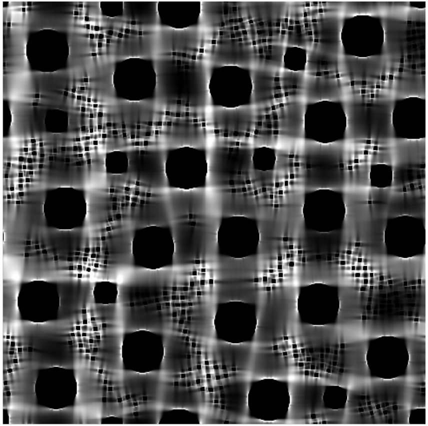
$$\overline{w}(\overline{\varepsilon}) = \sum_{r=1}^{N} c^{(r)} \left[w^{(r)}(\langle\varepsilon\rangle^{(r)}) + \frac{1}{2}\frac{\partial w^{(r)}}{\partial \varepsilon}\left(\langle\varepsilon\rangle^{(r)}\right) \cdot \left(\overline{\varepsilon} - \langle\varepsilon\rangle^{(r)}\right)\right]$$

- The estimate is not a bound (we don't know the sign of the error)
- The estimate depends on microstructural morphology ✓
- The estimate *is exact to second order in the heterogeneity contrast* ✓
- The estimate is not convex and exhibits a duality gap ✗
- The estimate can violate bounds ✗
- The non-linear stress-strain relation is not that of the linear-comparison composite; same with field statistics (Idiart and Ponte Castañeda, 2007) ✗

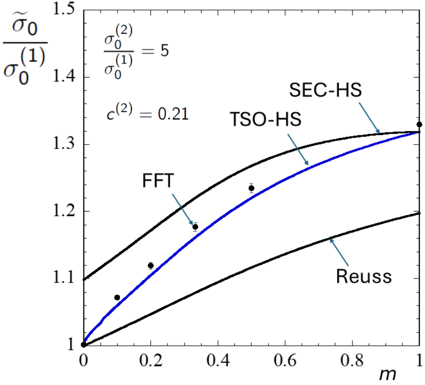
$$\overline{\boldsymbol{\sigma}} = \frac{\partial \overline{w}}{\partial \overline{\varepsilon}}(\overline{\varepsilon}) \neq \frac{\partial \overline{w}_c}{\partial \overline{\varepsilon}}(\overline{\varepsilon}; \boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)})$$

- We can use the linear-comparison composite as an estimate; it is the 'affine' estimate of Masson, Bornert, Suquet and Zaoui (2000), but it doesn't derive from an energy
- An alternative version of the estimate whose non-linear and linear-comparison relations coincide was proposed by Lahellec and Suquet (2004), but unfortunately inherits other innaccuracies

Tangent second-order estimates for power-law composites



strain distribution in a fiber-reinforced composite under simple shear when $m = 0.1$



Idiart, Moulinec, Ponte Castañeda and Suquet (2006)

Outline

1. The homogenized response $\rightarrow$ effective energy $\checkmark$
2. Elementary bounds on the effective energy $\checkmark$
3. Linear-comparison bounds on the effective energy $\checkmark$
4. Weak-contrast expansion of the effective energy $\checkmark$
5. Linear-comparison estimates of the effective energy $\sim$

Generalized-secant second-order estimates

Ponte Castañeda (2002) proposed the use of the alternative representation

$$w^{(r)}(\varepsilon) = \operatorname*{stat}_{\mathbb{C}^{(r)}} \left\{ \frac{1}{2}\varepsilon \cdot \mathbb{C}^{(r)}\varepsilon + \boldsymbol{\tau}^{(r)} \cdot \varepsilon + v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right) \right\}$$

and therefore the estimate

$$\overline{w}(\overline{\varepsilon}) = \min_{\varepsilon \,\in\, \mathcal{K}(\overline{\varepsilon})} \sum_{r=1}^{N} c^{(r)} \left\langle w^{(r)}(\varepsilon) \right\rangle^{(r)} \approx \operatorname*{stat}_{\mathbb{C}^{(r)}} \left\{ \min_{\varepsilon \,\in\, \mathcal{K}(\overline{\varepsilon})} \sum_{r=1}^{N} c^{(r)} \left\langle \frac{1}{2}\varepsilon \cdot \mathbb{C}^{(r)}\varepsilon + \boldsymbol{\tau}^{(r)} \cdot \varepsilon + v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right) \right\rangle^{(r)} \right\}$$

with the polarization still given by

$$\boldsymbol{\tau}^{(r)} = \frac{\partial w^{(r)}}{\partial \varepsilon}(\breve{\varepsilon}^{(r)}) - \mathbb{C}^{(r)}\breve{\varepsilon}^{(r)}$$

but with the reference strain $\breve{\varepsilon}^{(r)}$ to be chosen ad-hoc.

Generalized-secant second-order estimates

Experience with the tangent second-order estimate suggests the choice

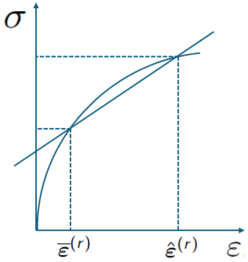
$$\breve{\varepsilon}^{(r)} = \langle \varepsilon \rangle^{(r)} \equiv \overline{\varepsilon}^{(r)}$$

Stationarity conditions require that

$$\frac{\partial w^{(r)}}{\partial \varepsilon}(\hat{\varepsilon}^{(r)}) - \frac{\partial w^{(r)}}{\partial \varepsilon}(\overline{\varepsilon}^{(r)}) = \mathbb{C}^{(r)}\left(\hat{\varepsilon}^{(r)} - \overline{\varepsilon}^{(r)}\right)$$

and that (traces of)

$$\left(\hat{\varepsilon}^{(r)} - \overline{\varepsilon}^{(r)}\right) \otimes \left(\hat{\varepsilon}^{(r)} - \overline{\varepsilon}^{(r)}\right) = \left\langle \left(\varepsilon - \overline{\varepsilon}^{(r)}\right) \otimes \left(\varepsilon - \overline{\varepsilon}^{(r)}\right)\right\rangle^{(r)}$$



Generalized secant linearization

Generalized-secant second-order estimates

- The final expression for the estimate can be written as (Ponte Castañeda, 2002)

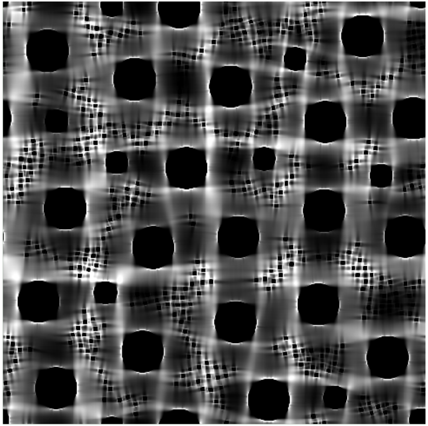
$$\overline{w}(\overline{\varepsilon}) = \sum_{r=1}^{N} c^{(r)} \left[w^{(r)}(\hat{\varepsilon}^{(r)}) - \frac{\partial w^{(r)}}{\partial \varepsilon}(\overline{\varepsilon}^{(r)}) \cdot \left(\hat{\varepsilon}^{(r)} - \overline{\varepsilon}^{(r)} \right) \right]$$

- The estimate is not a bound (we don't know the sign of the error)
- The estimate depends on microstructural morphology ✓
- The estimate *is exact to second order in the heterogeneity contrast* ✓
- The estimate is not convex and exhibits a duality gap in general ✗
- The estimate seems to satisfy bounds ✓
- The non-linear stress-strain relation is not that of the linear-comparison composite; same with field statistics (Idiart and Ponte Castañeda, 2007) ✗

$$\overline{\boldsymbol{\sigma}} = \frac{\partial \overline{w}}{\partial \overline{\boldsymbol{\varepsilon}}}(\overline{\boldsymbol{\varepsilon}}) \neq \frac{\partial \overline{w}_c}{\partial \overline{\boldsymbol{\varepsilon}}}(\overline{\boldsymbol{\varepsilon}}; \boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)})$$

- We can use the linear-comparison composite as an estimate; it is a generalization of the 'affine' estimate of Masson, Bornert, Suquet and Zaoui (2000) that incorporates second moments, see also Brenner, Castelnau and Gilormini (2001)
- The linear-comparison composite may become negative-definite; a possible remedy has been proposed by Idiart and Ponte Castañeda (2005)

Generalized-secant estimates for power-law composites



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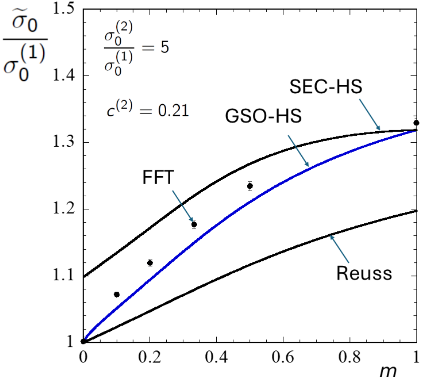
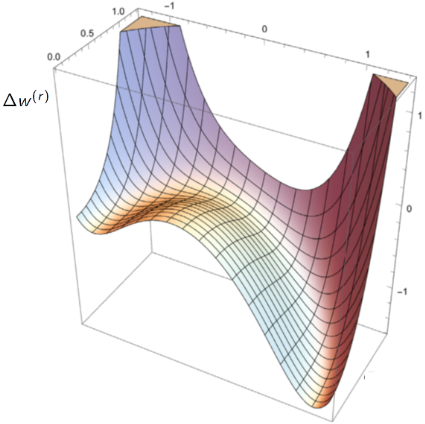
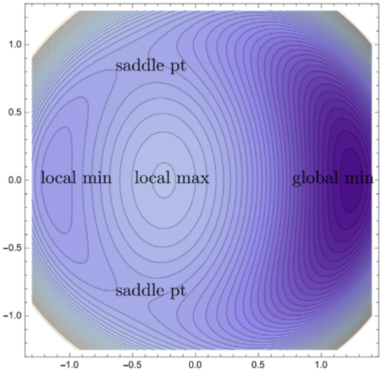


Idiart, Moulinec, Ponte Castañeda and Suquet (2006)

Generalized-secant second-order estimates

$$v^{(r)}\left(\boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)}\right) = \underset{\boldsymbol{\varepsilon}}{\text{stat}} \left\{ w^{(r)}(\boldsymbol{\varepsilon}) - \frac{1}{2}\boldsymbol{\varepsilon} \cdot \mathbb{C}^{(r)}\boldsymbol{\varepsilon} - \boldsymbol{\tau}^{(r)} \cdot \boldsymbol{\varepsilon} \right\}$$





Generalized-secant second-order estimates

Motivated by the previous observations, Ponte Castañeda (2016) proposed the use of the alternative representation

$$w^{(r)}(\boldsymbol{\varepsilon}) = \underset{\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}}{\text{stat}} \left\{ \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} + \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} + \alpha^{(r)}\check{v}^{(r)}\left(\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}\right) + (1-\alpha^{(r)})\hat{v}^{(r)}\left(\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}\right) \right\}$$

with $0 \leq \alpha^{(r)} \leq 1$, and therefore the estimate

$$\overline{w}(\overline{\boldsymbol{\varepsilon}}) = \min_{\boldsymbol{\varepsilon}\,\in\,\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \sum_{r=1}^{N} c^{(r)} \left\langle w^{(r)}(\boldsymbol{\varepsilon}) \right\rangle^{(r)} \approx \underset{\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}}{\text{stat}} \left\{ \min_{\boldsymbol{\varepsilon}\,\in\,\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \sum_{r=1}^{N} c^{(r)} \left\langle \frac{1}{2}\boldsymbol{\varepsilon}\cdot\mathbb{C}^{(r)}\boldsymbol{\varepsilon} + \boldsymbol{\tau}^{(r)}\cdot\boldsymbol{\varepsilon} + v^{(r)}\left(\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}\right) \right\rangle^{(r)} \right\}$$

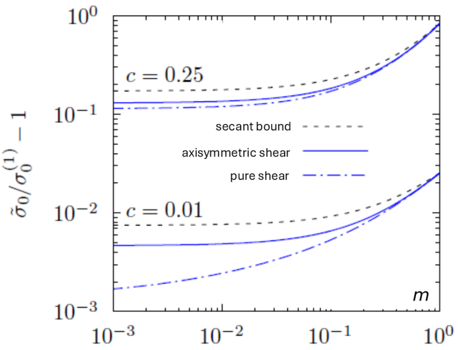
with

$$v^{(r)}\left(\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}\right) = \alpha^{(r)}\check{v}^{(r)}\left(\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}\right) + (1-\alpha^{(r)})\hat{v}^{(r)}\left(\boldsymbol{\tau}^{(r)},\mathbb{C}^{(r)}\right)$$

Experience and certain theoretical considerations suggest the choice $\alpha^{(r)} = 1/2$ (Furer, Idiart, Ponte Castañeda, 2020)

Generalized-secant estimates for power-law composites

Kammer and Ponte Castañeda (2024) carried out calculations for composites reinforced with spherical particles using the Hashin-Shtrikman estimates for the linear-comparison composite.



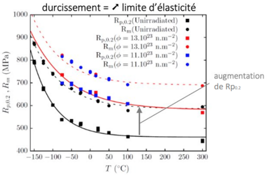
Generalized-secant second-order estimates

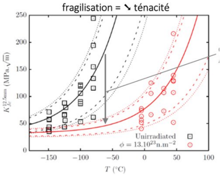
- The estimate is not a bound (we don't know the sign of the error)
- The estimate depends on microstructural morphology ✓
- The estimate *is exact to second order in the heterogeneity contrast* ✓
- The estimate exhibits no duality gap (Furer and Ponte Castañeda, 2017); is it convex?
- The estimate seems to satisfy bounds ✓
- The non-linear stress-strain relation coincides with that of the linear-comparison composite ✓

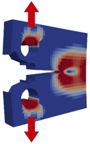
$$\overline{\boldsymbol{\sigma}} = \frac{\partial \overline{w}}{\partial \overline{\boldsymbol{\varepsilon}}}(\overline{\boldsymbol{\varepsilon}}) = \frac{\partial \overline{w}_c}{\partial \overline{\boldsymbol{\varepsilon}}}(\overline{\boldsymbol{\varepsilon}}; \boldsymbol{\tau}^{(r)}, \mathbb{C}^{(r)})$$

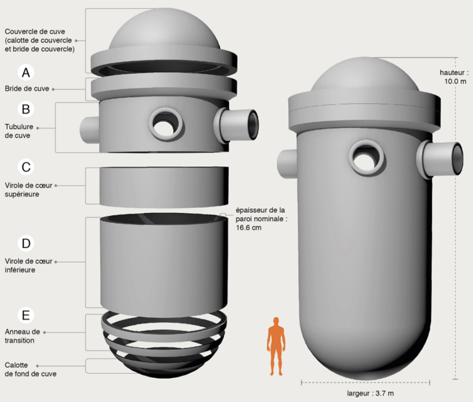
- Calculations become (excessively?) more involved (Kammer and Ponte Castañeda, 2024) ✗
- Ideas conducing to simpler estimates currently under investigation (e.g., Idiart, Chaix, Ponte Castañeda, 2024)

Application: bainitic steels under irradiation





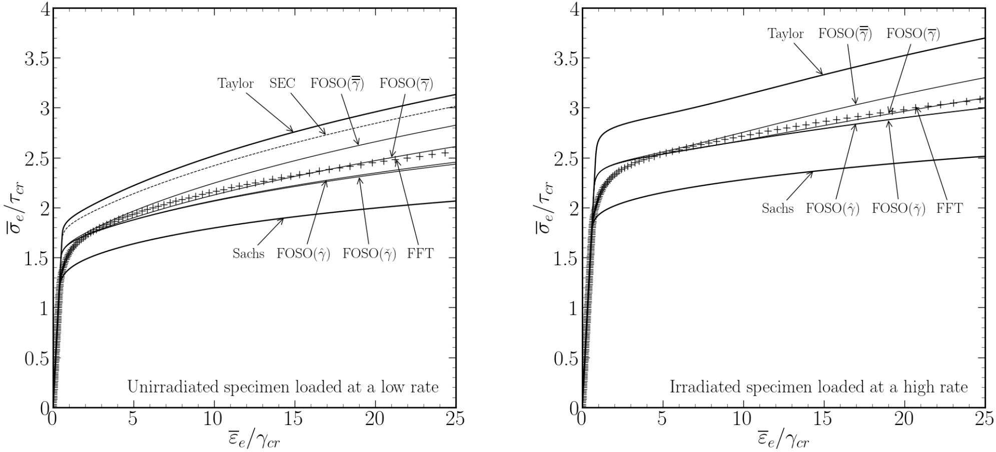




- Crystal plasticity law proposed by Monnet et al. (2019)
- Homogenized description for polycrystal by FOSO + Self-Consistent approx.

Chaix, Garajeu, Vincent, Monnet, Idiart (2024)

Application: sub-freezing temperatures



Chaix, Garajeu, Vincent, Monnet, Idiart (2024)

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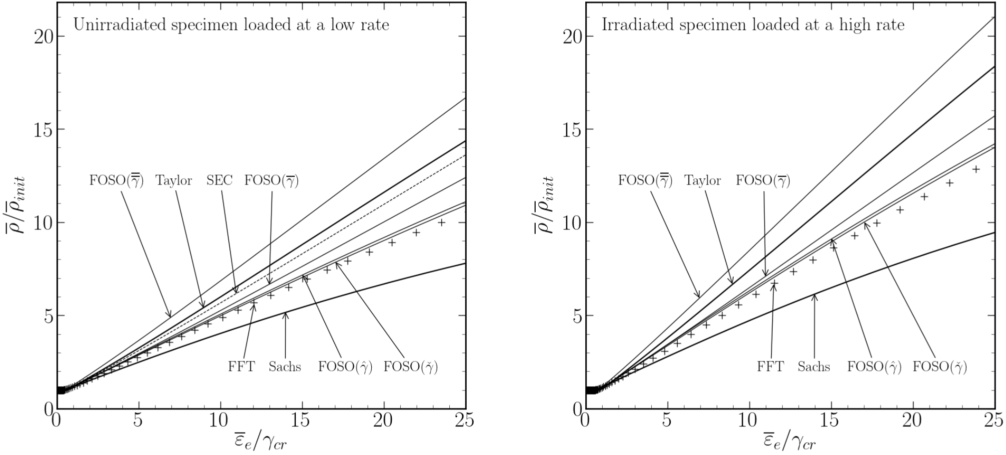

Chaix, Garajeu, Vincent, Monnet, Idiart (2024)

Summary

- Variational formulations can be employed to develop non-linear homogenization methods relying on linear-comparison composites optimally chosen
- Different formulations generate different linearizations (secant, tangent, generalized secant) with pros and cons
- An ideal formulation is yet to come... nice challenge for doctoral students and post-doctoral researchers...

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- Meanwhile, available formulations can handle already a wide range of material systems even with strong nonlinearities
- For complicated systems (e.g., viscoplastic polycrystals) estimates can be quite complicated $\rightarrow$ boost by machine learning (e.g., Ochoa, 2018; Tannous, Ghnatios, Castelnau, Ponte Castañeda, Chinesta, 2025)

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- Other strategies have also been put forward (e.g., Bornert, Stolz and Zaoui, 1996; Milton and Serkov, 2000; Pellegrini, 2001; Idiart, 2008, Michel and Suquet 2017,...)