Few notes on mean-field homogenization methods, and on the python code pyMFH

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1 The python code pyMFH

pyMFH stands for 'python Mean Field Homogenization'. The code is written for Thermo-Elastic local behavior in a context of general local and effective anisotropies. It will be extend to nonlinear behavior soon.

1.1 Notation convention used in the code

- `A33` for a tensor of rank 2 with indexes i, j in range 1 to 3
- `A6` the same tensor as `A33` but represented by a vector with index i in range 1 to 6
- `sig33` is the mean local stress (i.e. phase average), `sigbar33` is the effective stress, `sig233` is the second moment of the local stress tensor computed with a mechanical phase, `sigSD` is the associated standard deviation.
- `bar` or `eff` are for the mean or effective tensors, all other variables are local quantities.

2 General relations

For a *purely elastic* problem:

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} \ , \qquad \bar{\boldsymbol{\sigma}} = \tilde{\mathbf{C}} : \bar{\boldsymbol{\varepsilon}} \tag{1}$$

with

$$\boldsymbol{\varepsilon} = \mathbf{A} : \bar{\boldsymbol{\varepsilon}} \ , \qquad \boldsymbol{\sigma} = \mathbf{B} : \bar{\boldsymbol{\sigma}} \ , \qquad \langle \mathbf{A} \rangle = \langle \mathbf{B} \rangle = \mathbf{I} \tag{2}$$

and

$$\tilde{\mathbf{C}} = \langle \mathbf{C} : \mathbf{A} \rangle \ , \qquad \tilde{\mathbf{S}} = \langle \mathbf{S} : \mathbf{B} \rangle \tag{3}$$

leading to

$$\mathbf{A} = \mathbf{C}^{-1} : \mathbf{B} : \tilde{\mathbf{C}} \ , \qquad \mathbf{B} = \mathbf{C} : \mathbf{A} : \tilde{\mathbf{C}}^{-1} \ . \tag{4}$$

For a *thermo-elastic* behavior,

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\mathrm{el}} + \boldsymbol{\varepsilon}^{0} = \mathbf{S} : \boldsymbol{\sigma} + \boldsymbol{\varepsilon}^{0} \ , \tag{5}$$

$$\boldsymbol{\sigma} = \mathbf{B} : \bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}^{\mathrm{res}} = \mathbf{C} : (\varepsilon - \varepsilon^{0}) \ , \qquad \langle \boldsymbol{\sigma}^{\mathrm{res}} \rangle = \mathbf{0} \tag{6}$$

and

$$\bar{\varepsilon} = \tilde{\mathbf{S}} : \bar{\boldsymbol{\sigma}} + \tilde{\varepsilon}^{0} \ , \qquad \tilde{\varepsilon}^{0} = \left\langle \boldsymbol{\varepsilon}^{0} : \mathbf{B} \right\rangle \tag{7}$$

with the same strain localization and stress concentration tensors as for the purely elastic case.

3 Thermo-elastic Reuss and Voigt bounds

3.1 Reuss bound

$$\mathbf{B} = \mathbf{I} \,, \qquad \mathbf{A} = \mathbf{C}^{-1} : \tilde{\mathbf{C}} \,, \qquad \tilde{\mathbf{S}} = \langle \mathbf{S} \rangle \,, \qquad \tilde{\boldsymbol{\varepsilon}}^0 = \left\langle \boldsymbol{\varepsilon}^0 \right\rangle \,. \tag{8}$$

Stress uniformity means that

$$\boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}} \,, \qquad \boldsymbol{\sigma}^{\mathrm{res}} = \mathbf{0} \,. \tag{9}$$

3.2 Voigt bound

$$\mathbf{A} = \mathbf{I} \,, \qquad \mathbf{B} = \mathbf{C} : \tilde{\mathbf{C}}^{-1} \,, \qquad \tilde{\mathbf{C}} = \langle \mathbf{C} \rangle \,, \qquad \tilde{\boldsymbol{\varepsilon}}^0 = \left\langle \boldsymbol{\varepsilon}^0 : \mathbf{C} \right\rangle : \tilde{\mathbf{C}}^{-1} \,. \tag{10}$$

Strain uniformity for purely thermal loading leads to

$$\boldsymbol{\varepsilon}^{\mathrm{th}} = \tilde{\boldsymbol{\varepsilon}}^0 \tag{11}$$

so that

$$\boldsymbol{\sigma}^{\mathrm{res}} = \mathbf{C} : (\tilde{\boldsymbol{\varepsilon}}^0 - \boldsymbol{\varepsilon}^0) \,. \tag{12}$$

4 Mechanical response of a thermo-elastic laminate

Consider a n-phase laminate with $\mathbf{n}$ denoting the unit vector normal to the layer interfaces. see Faurie et al. JAC 2009 and references therein. Also He et al. 2012 mais il y a des erreurs dans le papier de He (sur la partie thermoelastique). Et bien sur Milton. Citer aussi le papier initial en geophys (ref ?).

4.1 Purely elastic response

According to Milton (*Theory of composites*, Cambridge University Press, 2002, see §9.5 page 167), the effective elastic behavior of a laminate composite made of a periodic arrangement of infinite parallel layers reads

$$\left[\sigma_0(\sigma_0\mathbf{I} - \tilde{\mathbf{C}})^{-1} - \boldsymbol{\Gamma}_1(\mathbf{n})\right]^{-1} =< \left[\sigma_0(\sigma_0\mathbf{I} - \mathbf{C})^{-1} - \boldsymbol{\Gamma}_1(\mathbf{n})\right]^{-1} > \tag{13}$$

with σ_0 an arbitrary scalar[1], $\mathbf{I}$ the fourth order identity tensor with components $I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, $\tilde{\mathbf{C}}$ the effective stiffness of the composite, $\mathbf{C}$ the (uniform) stiffness of each layer, and $< . >$ denoting the volume average over the whole specimen Ω. It is worth noting that the above relation is *exact*, and holds for general anisotropy of the layers. $\boldsymbol{\Gamma}_1$ is a purely geometrical tensor, depending only on the normal $\mathbf{n}$ of the layer surface. Its components read

$$[\boldsymbol{\Gamma}_1(\mathbf{n})]_{ijlm} = \frac{1}{2}(n_i\delta_{jl}n_m + n_i\delta_{jm}n_l + n_j\delta_{il}n_m + n_j\delta_{im}n_l) - n_i n_j n_l n_m. \tag{14}$$

$\boldsymbol{\Gamma}_1$ exhibits minor and major symetries, i.e. $[\boldsymbol{\Gamma}_1]_{ijlm} = [\boldsymbol{\Gamma}_1]_{jilm} = [\boldsymbol{\Gamma}_1]_{ijml} = [\boldsymbol{\Gamma}_1]_{lmij}$. The above result is independent of the precise arrangement of the layers. It only depends on their relative volume fraction.

[1] σ_0 is taken of the same order of magnitude as $\mathbf{C}$ in the numerical calculations.

A remarkable result is that, for homogeneous boundary conditions, the stress and strain are *uniform* in each layer. For example, if $\mathbf{n} \equiv \mathbf{e}_3$, then $\sigma_{i3}(\mathbf{x}) = \bar{\sigma}_{i3}$ $(i = 1, 3)$ and $\varepsilon_{kl}(\mathbf{x}) = \bar{\varepsilon}_{kl}$ $(k, l = 1, 2)$ for all $\mathbf{x} \in \Omega$, with $\bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{\varepsilon}}$ denoting the effective stress and strain, respectively, and $\boldsymbol{\sigma}(\mathbf{x})$ and $\boldsymbol{\varepsilon}(\mathbf{x})$ the corresponding local quantities at point $\mathbf{x}$. It can be verified that $\boldsymbol{\Gamma}_1$ extracts the corresponding components of $\bar{\boldsymbol{\sigma}}$

$$\boldsymbol{\Gamma}_1 : \boldsymbol{\sigma} = (\boldsymbol{\sigma}.\mathbf{n}) \otimes \mathbf{n} + \mathbf{n} \otimes (\boldsymbol{\sigma}.\mathbf{n}) - (\mathbf{n}.\boldsymbol{\sigma}.\mathbf{n})\mathbf{n} \otimes \mathbf{n}. \tag{15}$$

Similarly, a second operator $\boldsymbol{\Gamma}_2$ can be define to extract the corresponding component of $\bar{\boldsymbol{\varepsilon}}$

$$\boldsymbol{\Gamma}_2 = \mathbf{I} - \boldsymbol{\Gamma}_1. \tag{16}$$

It is thus true that

$$\forall \mathbf{x} \in \Omega, \quad \boldsymbol{\Gamma}_1 : \boldsymbol{\sigma}(\mathbf{x}) = \boldsymbol{\Gamma}_1 : \bar{\boldsymbol{\sigma}}, \quad \text{and} \quad \boldsymbol{\Gamma}_2 : \boldsymbol{\varepsilon}(\mathbf{x}) = \boldsymbol{\Gamma}_2 : \bar{\boldsymbol{\varepsilon}}. \tag{17}$$

This last equation allows the determination of the stress localization tensor $\mathbf{B}(\mathbf{x})$, defined as the "ratio" between local stress $\boldsymbol{\sigma}(\mathbf{x})$ and applied stress $\bar{\boldsymbol{\sigma}}$

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{B}(\mathbf{x}) : \bar{\boldsymbol{\sigma}}. \tag{18}$$

Noting that the local constitutive relation can be written

$$(\boldsymbol{\Gamma}_1 + \boldsymbol{\Gamma}_2) : \boldsymbol{\sigma} = \mathbf{C} : (\boldsymbol{\Gamma}_1 + \boldsymbol{\Gamma}_2) : \boldsymbol{\varepsilon}, \tag{19}$$

and using $\boldsymbol{\varepsilon} = \mathbf{S} : \mathbf{B} : \bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{\varepsilon}} = \tilde{\mathbf{S}} : \bar{\boldsymbol{\sigma}}$, it is easy to show that

$$\mathbf{B}(\mathbf{x}) = -(\boldsymbol{\Gamma}_2 - \mathbf{C} : \boldsymbol{\Gamma}_1 : \mathbf{S})^{-1} : (\boldsymbol{\Gamma}_1 - \mathbf{C} : \boldsymbol{\Gamma}_2 : \tilde{\mathbf{S}}) \tag{20}$$

which identically reads

$$\mathbf{B}(\mathbf{x}) = (\boldsymbol{\Gamma}_1 : \mathbf{S} - \mathbf{S} : \boldsymbol{\Gamma}_2)^{-1} : (\mathbf{S} : \boldsymbol{\Gamma}_1 - \boldsymbol{\Gamma}_2 : \tilde{\mathbf{S}})\ . \tag{21}$$

Similarly, one gets the strain localisation tensor, using $\boldsymbol{\varepsilon} = \mathbf{A} : \tilde{\varepsilon}$

$$\mathbf{A}^{(r)} = \left[\boldsymbol{\Gamma}^{(2)} : \mathbf{C}^{(r)} - \mathbf{C}^{(r)} : \boldsymbol{\Gamma}^{(1)}\right]^{-1} : \left[\mathbf{C}^{(r)} : \boldsymbol{\Gamma}^{(2)} - \boldsymbol{\Gamma}^{(1)} : \tilde{\mathbf{C}}\right]\ . \tag{22}$$

They are such that

$$\langle \mathbf{A} \rangle = \langle \mathbf{B} \rangle = \mathbf{I}\ . \tag{23}$$

and

$$\tilde{\mathbf{C}} = \langle \mathbf{C} : \mathbf{A} \rangle\ , \qquad \tilde{\mathbf{S}} = \langle \mathbf{S} : \mathbf{B} \rangle\ . \tag{24}$$

4.2 Thermo-elastic response

We consider now the case for which the phases exihibit some (stress-free) thermal strain,

$$\boldsymbol{\varepsilon}^0 = \boldsymbol{\alpha}\Delta T \tag{25}$$

with $\boldsymbol{\alpha}$ the (anisotropic) local dilation modulus and ΔT the temperature change. The local behavior is thus given by

$$\boldsymbol{\varepsilon} = \mathbf{S} : \boldsymbol{\sigma} + \boldsymbol{\varepsilon}^0\ , \qquad \boldsymbol{\sigma} = \mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^0)\ , \qquad \boldsymbol{\sigma} = \mathbf{B} : \bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}^{res} \tag{26}$$

with $\mathbf{B}$ the stress concentration tensor of the purely elastic problem (see previous section) and $\boldsymbol{\sigma}^{res}$ the field of residual stress, which is homogeneous per phase. The elastic strain is

$$\boldsymbol{\varepsilon}^e = \mathbf{S} : \boldsymbol{\sigma} \tag{27}$$

and is due partly to the thermal loading and partly to the applied macroscopic stress. The effective behavior is given by

$$\bar{\boldsymbol{\varepsilon}} = \tilde{\mathbf{S}} : \bar{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\varepsilon}}^0 \ . \tag{28}$$

where the effective compliance $\tilde{\mathbf{S}}$ is identical to the one for the purely elastic case (previous section) while the effective stress-free strain is

$$\tilde{\boldsymbol{\varepsilon}}^0 = \left\langle \boldsymbol{\varepsilon}^0 : \mathbf{B} \right\rangle \ . \tag{29}$$

It is composed of the thermal strain $\boldsymbol{\varepsilon}^0$, which is incompatible, and an elastic strain necessary to render the total strain $\boldsymbol{\varepsilon}$ compatible.

To express the residual stress in each phase, one has to remark that (17) combined with (16) leads to

$$\boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} + \boldsymbol{\Gamma}^1 : (\boldsymbol{\varepsilon} - \bar{\boldsymbol{\varepsilon}}) \ , \qquad \boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}} + \boldsymbol{\Gamma}^2 : (\boldsymbol{\sigma} - \bar{\boldsymbol{\sigma}}) \ . \tag{30}$$

These latter expressions can be plugged into the local behavior $(26)_2$ to give

$$\left(\mathbf{S} : \boldsymbol{\Gamma}^2 - \boldsymbol{\Gamma}^1 : \mathbf{S}\right) : \boldsymbol{\sigma} = \boldsymbol{\Gamma}^2 : (\bar{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}^0) - \mathbf{S} : \boldsymbol{\Gamma}^1 : \bar{\boldsymbol{\sigma}} \ . \tag{31}$$

The residual stress is defined as the field of stress remaining in the material when there is no applied stress, i.e. for $\bar{\boldsymbol{\sigma}} = \mathbf{0}$ leading also to $\bar{\boldsymbol{\varepsilon}} = \tilde{\boldsymbol{\varepsilon}}^0$. One thus gets

$$\boldsymbol{\sigma}^{res} = \left(\mathbf{S} : \boldsymbol{\Gamma}^2 - \boldsymbol{\Gamma}^1 : \mathbf{S}\right)^{-1} : \boldsymbol{\Gamma}^2 : (\tilde{\boldsymbol{\varepsilon}}^0 - \boldsymbol{\varepsilon}^0) \ . \tag{32}$$

4.3 Some analytical expressions

- voir aussi le TD dans CE2M10, pour les qq resultats analytiques.
- Make use of Levine relation in case of 2-phases laminate ?