Homogenization based on realization-dependent Hashin-Shtrikman functionals of piecewise polynomial trial polarization fields

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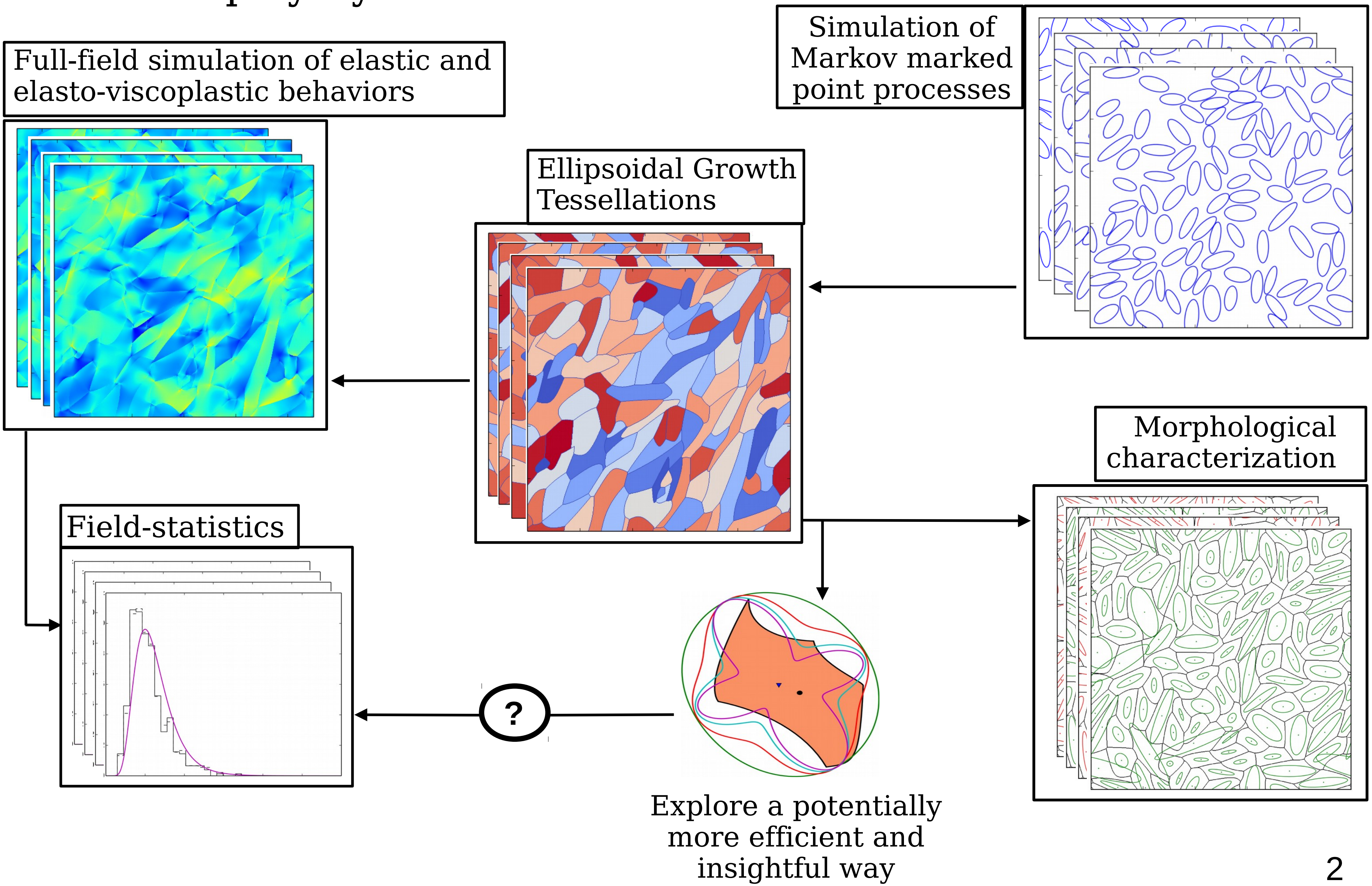
Motivation/Objective

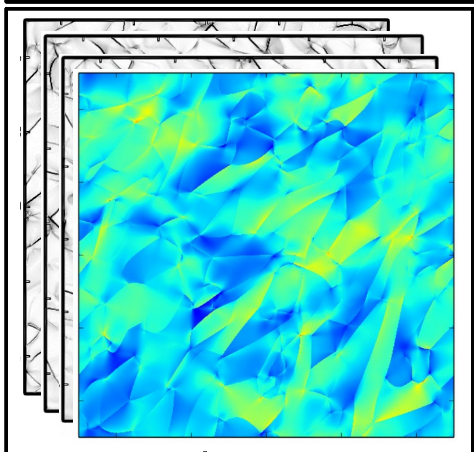
- Understand the role of morphology on the mechanical performance of random polycrystals



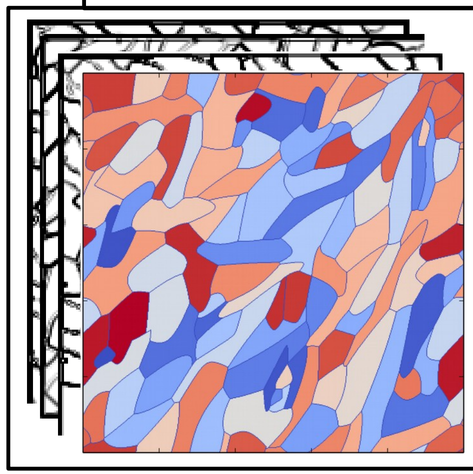
Motivation/Objective

- Understand the role of morphology on the mechanical performance of random polycrystals

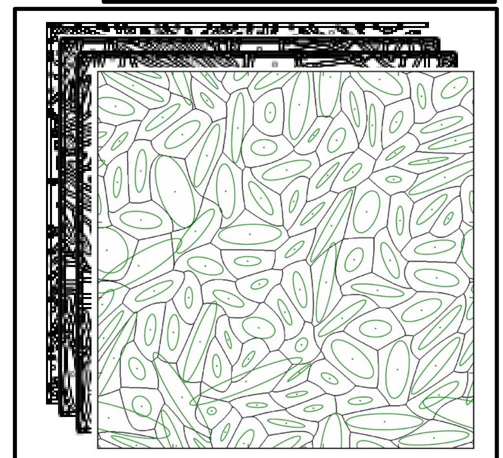
Full-field simulation of elastic and elasto-viscoplastic behaviors



Ellipsoidal Growth Tessellations



Morphological characterization



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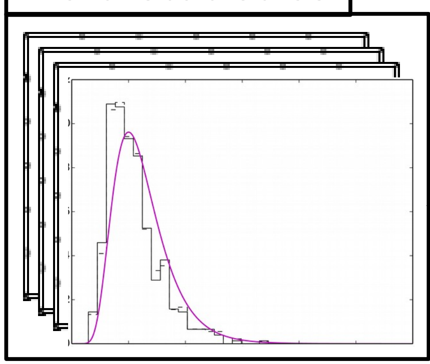
Field-statistics



On a ***realization-by-realization*** basis, can we

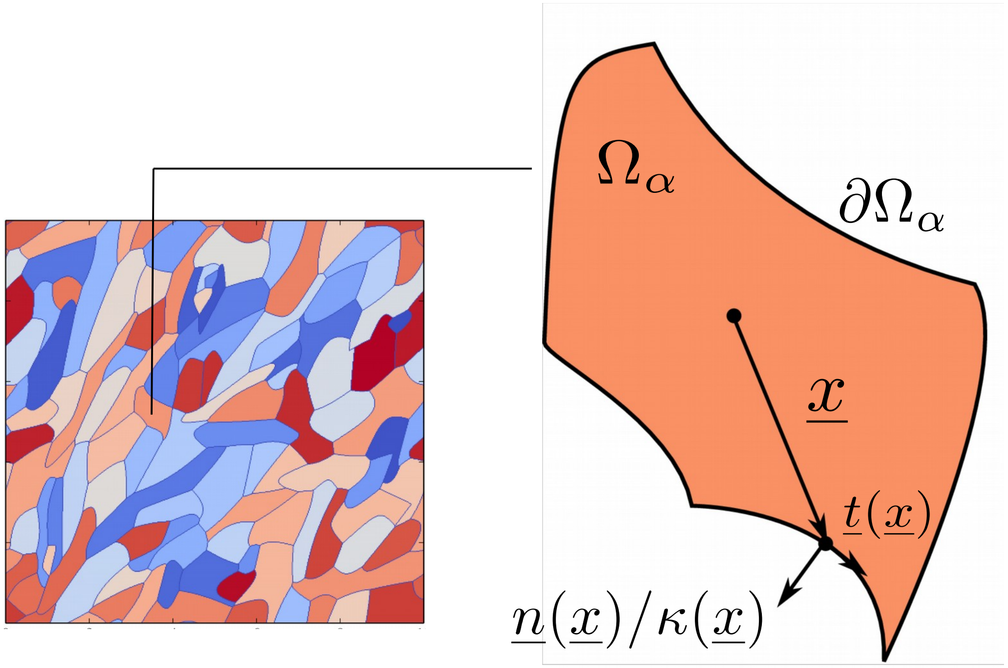
Define ***micromechanical schemes*** that use information about

- Morphological symmetry/anisotropy
- Material symmetry and constitutive behavior

to *estimate field statistics* of mechanical behaviors *efficiently* and *accurately enough?*

Morphological characterization

Single grains are characterized using Minkowski tensors:



Measures of mass distribution:

$$\mathcal{W}_0^{r,0} = \int_{\Omega_\alpha} \underline{x}^{\otimes^r} \mathrm{d}V$$

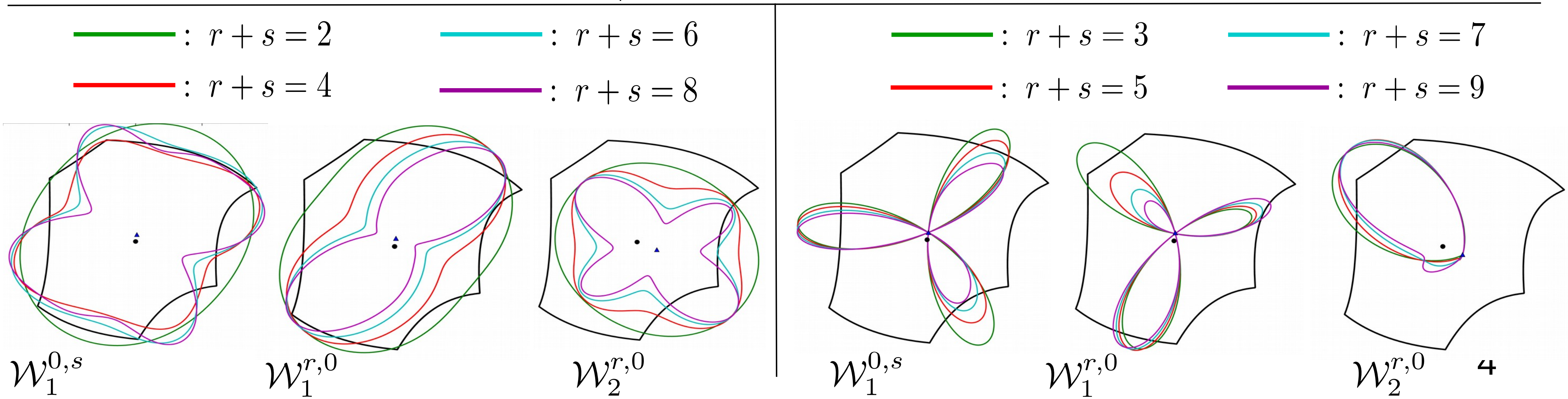
Measures of surface distribution:

$$\mathcal{W}_1^{r,s} = \int_{\partial\Omega_\alpha} \underline{x}^{\otimes^r} \odot [\underline{n}(\underline{x})]^{\otimes^s} \mathrm{d}S$$

Curvature-weighted measures of surface distribution:

$$\mathcal{W}_2^{r,s} = \int_{\partial\Omega_\alpha} \kappa(\underline{x})\underline{x}^{\otimes^r} \odot [\underline{n}(\underline{x})]^{\otimes^s} \mathrm{d}S$$

Reynolds glyphs of Minkowski tensors



Lippmann-Schwinger equation for periodic elastic media

Periodic elastic BVP:

$$\boldsymbol{\sigma}(\underline{x}) = \mathbb{L}(\underline{x}) : \boldsymbol{\varepsilon}(\underline{x}) \,, \qquad \nabla \cdot \boldsymbol{\sigma}(\underline{x}) = \underline{0} \,, \qquad \boldsymbol{\varepsilon}(\underline{x}) = \{\nabla \underline{u}(\underline{x})\}_{sym}$$

for all $\underline{x} \in \mathbb{R}^2$, with $\mathbb{L}(\underline{x} + (n\underline{e}_1 + m\underline{e}_2)L) = \mathbb{L}(\underline{x})$ for all $n, m \in \mathbb{Z}$ s.t.

$$\underline{u}(\underline{x} + (n\underline{e}_1 + m\underline{e}_2)L) = \underline{u}(\underline{x}) + L\,\overline{\boldsymbol{\varepsilon}} \cdot (n\underline{e}_1 + m\underline{e}_2)$$

$$\boldsymbol{\sigma}(\underline{x} + (n\underline{e}_1 + m\underline{e}_2)) \cdot \underline{e}_k = \boldsymbol{\sigma}(\underline{x}) \cdot \underline{e}_k \text{ for } k = 1, 2$$

and where $\overline{\bullet} := \dfrac{1}{L^2}\displaystyle\int_\Omega \bullet(\underline{x}) \mathrm{d}\nu_{\underline{x}}$ is a volume average over $\Omega := [0, L] \times [0, L]$.

Then, as we introduce the polarization field $\boldsymbol{\tau}$ with reference $\mathbb{L}^0$,

$$\boldsymbol{\tau}(\underline{x}) := \boldsymbol{\sigma}(\underline{x}) - \mathbb{L}^0 : \boldsymbol{\varepsilon}(\underline{x}) = \Delta\mathbb{L}(\underline{x}) : \boldsymbol{\varepsilon}(\underline{x})$$

where $\Delta\mathbb{L}(\underline{x}) := \mathbb{L}(\underline{x}) - \mathbb{L}^0$, the local statement of equilibrium becomes

$$\nabla \cdot \boldsymbol{\tau}(\underline{x}) + \nabla \cdot [\mathbb{L}^0 : \boldsymbol{\varepsilon}(\underline{x})] = \underline{0}$$

Disturbance strain field $\tilde{\varepsilon}(\underline{x})$ with vanishing field average.

with solution

$$\boldsymbol{\varepsilon}(\underline{x}) = \overline{\boldsymbol{\varepsilon}} - \boxed{\boldsymbol{\Gamma} * \boldsymbol{\tau}(\underline{x})} = \overline{\boldsymbol{\varepsilon}} - \boldsymbol{\Gamma} * [\Delta\mathbb{L} : \boldsymbol{\varepsilon}(\underline{x})]$$

Lippmann-Schwinger equation

in which $\boldsymbol{\Gamma} * \boldsymbol{\tau}(\underline{x}) := \displaystyle\int_{\mathbb{R}^2} \boldsymbol{\Gamma}(\underline{x}' - \underline{x}) : \boldsymbol{\tau}(\underline{x}') \, \mathrm{d}\nu_{\underline{x}'}.$

Periodic Green operator for strains.

Note that for all $\underline{x}$, we have $\overline{\boldsymbol{\varepsilon}} = [\Delta\mathbb{L}(\underline{x})]^{-1} : \boldsymbol{\tau}(\underline{x}) + \boldsymbol{\Gamma} * \boldsymbol{\tau}(\underline{x})$

Hashin-Shtrikman (HS) variational principle

Multiplying the previous expression by a test field $\boldsymbol{\tau}'$, we have

$$\boldsymbol{\tau}'(\underline{x}) : \overline{\boldsymbol{\varepsilon}} = \boldsymbol{\tau}'(\underline{x}) : [\Delta\mathbb{L}(\underline{x})]^{-1} : \boldsymbol{\tau}(\underline{x}) + \boldsymbol{\tau}'(\underline{x}) : (\boldsymbol{\Gamma} * \boldsymbol{\tau})(\underline{x})$$

which, after volume averaging over Ω, becomes

$$\overline{\boldsymbol{\tau}'} : \overline{\boldsymbol{\varepsilon}} = \overline{\boldsymbol{\tau}' : \Delta\mathbb{L}^{-1} : \boldsymbol{\tau}} + \overline{\boldsymbol{\tau}' : (\boldsymbol{\Gamma} * \boldsymbol{\tau})}$$

Differential of the HS functional evaluated at the equilibrated stress $\boldsymbol{\tau}$

The HS functional is defined as follows by Hashin and Shtrikman (1962):

$$\mathcal{H}(\boldsymbol{\tau}') := \overline{\boldsymbol{\tau}'} : \overline{\boldsymbol{\varepsilon}} - 1/2\,\overline{\boldsymbol{\tau}' : (\Delta\mathbb{L})^{-1} : \boldsymbol{\tau}'} - 1/2\,\overline{\boldsymbol{\tau}' : (\boldsymbol{\Gamma} * \boldsymbol{\tau}')}$$

$\mathcal{H}$ admits a *stationary state* for the equilibrated polarization field $\boldsymbol{\tau}$, *irrespectively of the reference stiffness* $\mathbb{L}^0$. *At equilibrium*, we also have $\mathcal{H}(\boldsymbol{\tau}) = 1/2\overline{\boldsymbol{\varepsilon}} : (\mathbb{L}^{eff} - \mathbb{L}^0) : \overline{\boldsymbol{\varepsilon}}$, where $\mathbb{L}^{eff}$ is s.t. $\overline{\boldsymbol{\sigma}} = \mathbb{L}^{eff} : \overline{\boldsymbol{\varepsilon}}$.

Boundedness conditions of $\mathcal{H}$:

$$\Delta\mathbb{L}(\underline{x}) \text{ PSD for all } \underline{x} \text{ implies } \mathcal{V}_1 \subseteq \mathcal{V}_2 \subseteq \mathcal{V} \implies \sup_{\mathcal{V}_1} \mathcal{H} \leq \sup_{\mathcal{V}_2} \mathcal{H} \leq \sup_{\mathcal{V}} \mathcal{H} = \mathcal{H}(\boldsymbol{\tau})$$

$$\Delta\mathbb{L}(\underline{x}) \text{ NSD for all } \underline{x} \text{ implies } \mathcal{V}_1 \subseteq \mathcal{V}_2 \subseteq \mathcal{V} \implies \inf_{\mathcal{V}_1} \mathcal{H} \geq \inf_{\mathcal{V}_2} \mathcal{H} \geq \inf_{\mathcal{V}} \mathcal{H} = \mathcal{H}(\boldsymbol{\tau})$$

Searching for polarization fields among richer functional spaces guarantees not to deteriorate the quality of the solution if the reference medium is chosen properly.

Case of piecewise constant polarization fields, i.e. $\mathcal{V}^{h_0}$

Assume $\boldsymbol{\tau}^{h_0}(\underline{x}) := \sum_{\alpha} \chi_\alpha(\underline{x})\boldsymbol{\tau}^{(\alpha)}$ where $\chi_\alpha := \begin{cases} 1 & \text{if } \underline{x} \in \Omega_\alpha \\ 0 & \text{otherwise} \end{cases}$.

Then $\overline{\boldsymbol{\tau}^{h_0} : (\boldsymbol{\Gamma} * \boldsymbol{\tau}^{h_0})} = \sum_{\alpha}\sum_{\gamma} \boldsymbol{\tau}^{\alpha} : \mathbb{T}^{\alpha\gamma}_{0,0} : \boldsymbol{\tau}^{\gamma}$, where

influence tensors

$$\boxed{\mathbb{T}^{\alpha\gamma}_{0,0} := \frac{1}{|\Omega|}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \chi_\alpha(\underline{x})\chi_\gamma(\underline{y})\boldsymbol{\Gamma}(\underline{x}-\underline{y})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}}}$$

so that the HS functional becomes

$$\mathcal{H}(\boldsymbol{\tau}) = \sum_{\alpha} c_\alpha \boldsymbol{\tau}^{\alpha} : \overline{\boldsymbol{\varepsilon}} - \frac{1}{2}\sum_{\alpha} c_\alpha \boldsymbol{\tau}^{\alpha} : (\Delta\mathbb{L}^{\alpha})^{-1} : \boldsymbol{\tau}^{\alpha} - \frac{1}{2}\sum_{\alpha}\sum_{\gamma} \boldsymbol{\tau}^{\alpha} : \mathbb{T}^{\alpha\gamma}_{0,0} : \boldsymbol{\tau}^{\gamma}$$

for which the stationary state is obtained for

$$c_\alpha(\Delta\mathbb{L}^{\alpha})^{-1} : \boldsymbol{\tau}^{\alpha} + \sum_{\gamma} \mathbb{T}^{\alpha\gamma}_{0,0} : \boldsymbol{\tau}^{\gamma} = c_\alpha \overline{\boldsymbol{\varepsilon}} \quad \text{for all } \alpha$$

Remark: We want to avoid integrating $\boldsymbol{\Gamma}$. Instead, we want to find a relation between $\mathbb{T}^{\alpha\gamma}_{0,0}$, the Minkowski tensors (which we use to characterize morphological anisotropy) of the microstructure, and the derivatives of $\boldsymbol{\Gamma}$.

Influence tensors for polarization fields in $\mathcal{V}^{h_0}$

To avoid singularities, we consider the domain $\Omega'_\alpha := \Omega_\alpha \uplus \{-\underline{x}_\alpha\}$ and let

$$\mathbb{T}^{\alpha\gamma}_{0,0} = \frac{1}{|\Omega|}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \chi_\alpha(\underline{x}+\underline{x}_{\gamma\alpha})\chi_\gamma(\underline{y}+\underline{x}_\gamma)\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}} = \frac{1}{|\Omega|}\int_{\Omega'_\gamma}\int_{\Omega'_\alpha} \boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}}$$

where $\underline{x}_{\gamma\alpha} := \underline{x}_\alpha - \underline{x}_\gamma$. Also, we consider the following Taylor expansion,

$${}^n\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) := \boldsymbol{\Gamma}(\underline{x}_{\gamma\alpha}) + \sum_{k=1}^{n}\sum_{i=0}^{k}\frac{(-1)^i}{(k-i)!i!}\left\langle \boldsymbol{\Gamma}^{(k)}(\underline{x}_{\gamma\alpha}), \underline{x}^{\otimes^{k-i}} \otimes \underline{y}^{\otimes^{i}} \right\rangle_k \text{ for all } (\underline{x},\underline{y}) \in \Omega'_\alpha \times \Omega'_\gamma$$

so that for $\gamma \neq \alpha$, we introduce the following estimates:

$${}^n\mathbb{T}^{\alpha\gamma}_{0,0} := \frac{1}{|\Omega|}\int_{\Omega'_\gamma}\int_{\Omega'_\alpha} {}^n\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}}$$

$${}^n\mathbb{T}^{\alpha\gamma}_{0,0} = c_\alpha c_\gamma |\Omega| \boldsymbol{\Gamma}(\underline{x}_{\gamma\alpha}) + \frac{1}{|\Omega|}\sum_{k=1}^{n}\sum_{i=0}^{k}\frac{(-1)^i}{(k-i)!i!}\left\langle \boldsymbol{\Gamma}^{(k)}(\underline{x}_{\gamma\alpha}), \mathcal{W}_0^{k-i,0}(\Omega'_\alpha)\otimes \mathcal{W}_0^{i,0}(\Omega'_\gamma)\right\rangle_k$$

where, $\boldsymbol{\Gamma}^{(m)}(\underline{x})$ is the *m*-th derivative of the Green operator, i.e. with components $\Gamma^{(m)}_{ijkln_1\ldots n_m}(\underline{x}) = \partial_{n_1\ldots n_m}\Gamma_{ijkl}(\underline{x})$.

Note that the Taylor expansion does satisfy the Maxwell-Betti theorem, i.e. for a stationary system

$${}^n\Gamma_{ijkl}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) = {}^n\Gamma_{klij}(\underline{y}-\underline{x}+\underline{x}_{\alpha\gamma})$$

Self-influence tensors for polarization fields in $\mathcal{V}^{h_0}$

When $\gamma = \alpha$, we refer to $\mathbb{T}_{0,0}^{\alpha\gamma}$ as a *self-influence* tensor. We can not integrate $\mathbf{\Gamma}(\underline{x} - \underline{y} + \underline{x}_{\alpha\alpha})$ over $\Omega'_\alpha \times \Omega'_\alpha$ because $\mathbf{\Gamma}$ is singular at the origin.

Instead, we proceed to the same change of variables as before, for some $\gamma \neq \alpha$. We obtain

$$\mathbb{T}_{0,0}^{\alpha\alpha} = \frac{1}{|\Omega|} \int_{\Omega_\alpha^\gamma} \int_{\Omega'_\alpha} \mathbf{\Gamma}(\underline{x} - \underline{y} + \underline{x}_{\gamma\alpha}) \mathrm{d}\nu_{\underline{x}} \mathrm{d}\nu_{\underline{y}}$$

where $\Omega_\alpha^\gamma := \Omega_\alpha \uplus \{-\underline{x}_\gamma\} = \{\underline{x} - \underline{x}_\gamma \mid \underline{x} \in \Omega_\alpha\}$. Using the same Taylor series expansion as before, we get

$${}^n\mathbb{T}_{0,0}^{\alpha\alpha} = c_\alpha^2 |\Omega| \mathbf{\Gamma}(\underline{x}_{\gamma\alpha}) + \frac{1}{|\Omega|} \sum_{k=1}^{n} \sum_{i=0}^{k} \frac{(-1)^i}{(k-i)!i!} \left\langle \mathbf{\Gamma}^{(k)}(\underline{x}_{\gamma\alpha}), \mathcal{W}_0^{k-i,0}(\Omega'_\alpha) \otimes \mathcal{W}_0^{i,0}(\Omega_\alpha^\gamma) \right\rangle_k$$

where, similarly, we have $\Omega_\alpha^\gamma = \Omega'_\alpha \uplus \{\underline{x}_{\gamma\alpha}\}$ so that $\mathcal{W}_0^{i,0}(\Omega_\alpha^\gamma) = \mathcal{W}_0^{i,0}(\Omega'_\alpha \{\underline{x}_{\gamma\alpha}\})$.

Because Minkowski tensors are motion covariant, we can write

$$\boxed{\mathcal{W}_0^{i,0}(\Omega_\alpha^\gamma) = \sum_{t=0}^{i} \binom{i}{t} \underline{x}_{\gamma\alpha}^{\otimes t} \odot \mathcal{W}_0^{i-t,0}(\Omega'_\alpha)}$$

Compute these for $i = 0, \ldots, n$

so that there is no need to re-analyze a digital microstructure to evaluate $\mathcal{W}_0^{i,0}(\Omega_\alpha^\gamma)$, which we need to compute the self-influence tensors.

Influence tensors for polarization fields in $\mathcal{V}^{h_0}$

To summarize, the following estimates of influence and self-influence tensors are obtained:

estimate of the 0-0 influence tensor of Ω_γ over Ω_α

$$ {}^n\mathbb{T}^{\alpha\gamma}_{0,0} := \frac{1}{|\Omega|}\int_{\Omega'_\gamma}\int_{\Omega'_\alpha} {}^n\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}} \qquad \gamma\neq\alpha $$

estimate of the 0-0 *self-influence tensor of* Ω_α

$$ {}^n\mathbb{T}^{\alpha\alpha}_{0,0} = \frac{1}{|\Omega|}\int_{\Omega^\gamma_\alpha}\int_{\Omega'_\alpha} {}^n\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}} \qquad \gamma\neq\alpha $$

which we respectively recast in the following expressions:

$$ ({}^nT^{\alpha\gamma}_{0,0})_{ijkl} = c_\alpha c_\gamma|\Omega|\Gamma_{ijkl}(\underline{x}_{\gamma\alpha}) + \sum_{k=1}^{n}\sum_{i=0}^{k}\frac{(-1)^i\Gamma^{(k)}_{ijklk_1..k_k}(\underline{x}_{\gamma\alpha})}{(k-i)!i!|\Omega|}[W_0^{k-i,0}(\Omega'_\alpha)]_{k_1..k_{k-i}}[W_0^{i,0}(\Omega'_\gamma)]_{k_{k-i+1}..k_k} $$

for all $\gamma\neq\alpha$

$$ \left.\begin{array}{l} {}^n\Gamma_{ijkl}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) = {}^n\Gamma_{klij}(\underline{y}-\underline{x}+\underline{x}_{\alpha\gamma}) \\ {}^n\Gamma_{ijkl}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) = {}^n\Gamma_{klij}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) \end{array}\right] \Longrightarrow ({}^nT^{\gamma\alpha}_{0,0})_{klij} = ({}^nT^{\gamma\alpha}_{0,0})_{ijkl} = ({}^nT^{\alpha\gamma}_{0,0})_{klij} = ({}^nT^{\alpha\gamma}_{0,0})_{ijkl} $$

$$ ({}^nT^{\alpha\alpha}_{0,0})_{ijkl} = c_\alpha^2|\Omega|\Gamma_{ijkl}(\underline{x}_{\gamma\alpha}) + \frac{1}{|\Omega|}\sum_{k=1}^{n}\sum_{i=0}^{k}\frac{(-1)^i\;{}^n\Gamma^{(k)}_{ijklk_1..k_k}(\underline{x}_{\gamma\alpha})}{(k-i)!i!}[W_0^{k-i,0}(\Omega'_\alpha)]_{k_1..k_{k-i}}[W_0^{i,0}(\Omega^\gamma_\alpha)]_{k_{k-i+1}..k_k} $$

for any $\gamma\neq\alpha$

For γ fixed, $({}^nT^{\alpha\alpha}_{0,0})_{ijkl} = ({}^nT^{\alpha\alpha}_{0,0})_{klij}$

Influence tensors for polarization fields in $\mathcal{V}^{h_0}$

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$$ {}^n\mathbb{T}^{\alpha\gamma}_{0,0} := \frac{1}{|\Omega|}\int_{\Omega'_\gamma}\int_{\Omega'_\alpha} {}^n\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}} $$

$\gamma \neq \alpha$

estimate of the 0-0 *self-influence tensor of* Ω_α

$$ {}^n\mathbb{T}^{\alpha\alpha}_{0,0} = \frac{1}{|\Omega|}\int_{\Omega^\gamma_\alpha}\int_{\Omega'_\alpha} {}^n\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}} $$

$\gamma \neq \alpha$

which we respectively recast in the following expressions:

$$ ({}^nT^{\alpha\gamma}_{0,0})_{ijkl} = c_\alpha c_\gamma |\Omega| \Gamma_{ijkl}(\underline{x}_{\gamma\alpha}) $$

$$ + \sum_{k=1}^{n}\sum_{i=0}^{k} \frac{(-1)^i \Gamma^{(k)}_{ijklk_1..k_k}(\underline{x}_{\gamma\alpha}\ldots}{(k-i)!i!|\Omega|} \ldots $$

for all $\gamma \neq \alpha$

$$ {}^n\Gamma_{ijkl}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) = {}^n\Gamma_{klij}(\underline{y}-\underline{x}+\underline{x}_{\alpha\gamma}) $$
$$ {}^n\Gamma_{ijkl}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) = {}^n\Gamma_{klij}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) $$
$\Longrightarrow$ $({}^nT^{\gamma\alpha}_{0,0} \ldots$

Results obtained for <u>piecewise constant</u> trial fields

$\Downarrow$

<u>No field statistics</u> available

$$ ({}^nT^{\alpha\alpha}_{0,0})_{ijkl} = c^2_\alpha |\Omega| \Gamma_{ijkl}(\underline{x}_{\gamma\alpha}) $$

$$ + \frac{1}{|\Omega|}\sum_{k=1}^{n}\sum_{i=0}^{k} \frac{(-1)^i\ {}^n\Gamma^{(k)}_{ijklk_1..k_k}(\underline{x}_{\gamma\alpha})}{(k-i)!i!} [W_0^{k-i,0}(\Omega'_\alpha)]_{k_1..k_{k-i}} [W_0^{i,0}(\Omega^\gamma_\alpha)]_{k_{k-i+1}..k_k} $$

for any $\gamma \neq \alpha$

For γ fixed, $({}^nT^{\alpha\alpha}_{0,0})_{ijkl} = ({}^nT^{\alpha\alpha}_{0,0})_{klij}$

Piecewise polynomial polarization fields, i.e. $\mathcal{V}^{h_p}$

Now, if we assume a trial polynomial field of degree p given by

$$\boldsymbol{\tau}^{h_p}(\underline{x}) := \sum_{\alpha} \left(\chi_\alpha(\underline{x}) \boldsymbol{\tau}^\alpha + \chi_\alpha(\underline{x}) \sum_{k=1}^{p} \left\langle \boldsymbol{\tau}^\alpha \boldsymbol{\partial}^k, (\underline{x} - \underline{x}^\alpha)^{\otimes^k} \right\rangle_k \right),$$

The term $\overline{\boldsymbol{\tau}^{h_p} : (\boldsymbol{\Gamma} * \boldsymbol{\tau}^{h_p})}$ then contains terms of the form

$$\int_{\Omega_\alpha} \int_{\Omega_\gamma} (x_{r_1} - x^\alpha_{r_1}) \ldots (x_{r_r} - x^\alpha_{r_r}) \Gamma_{ijkl}(\underline{x} - \underline{y})(y_{s_1} - x^\gamma_{s_1}) \ldots (y_{s_s} - x^\gamma_{s_s}) \mathrm{d}\nu_{\underline{x}} \mathrm{d}\nu_{\underline{y}}$$

$$= \quad \downarrow \text{Change of variable}$$

$$\int_{\Omega'_\alpha} \int_{\Omega'_\gamma} x_{r_1} \ldots x_{r_r} \Gamma_{ijkl}(\underline{x} - \underline{y} + \underline{x}_{\gamma\alpha}) y_{s_1} \ldots y_{s_s} \mathrm{d}\nu_{\underline{x}} \mathrm{d}\nu_{\underline{y}} \quad \text{where } \Omega'_\bullet := \{\underline{x} - \underline{x}_\bullet \mid \underline{x} \in \Omega_\bullet\}$$

which, similarly as before, can lead to estimates of "<u>r-s influence tensors of</u> Ω_γ <u>over</u> Ω_α"

$$({}^n T^{\alpha\gamma}_{r,s})_{r_1 \ldots r_r ijkl s_1 \ldots s_s} = \frac{1}{|\Omega|} [W_0^{r,0}(\Omega'_\alpha)]_{r_1 \ldots r_r} \Gamma_{ijkl}(\underline{x}_{\gamma\alpha}) [W_0^{s,0}(\Omega'_\gamma)]_{s_1 \ldots s_s}$$
$$+ \frac{1}{|\Omega|} \sum_{k=1}^{n} \sum_{i=0}^{k} \frac{(-1)^i}{(k-i)!i!} \Gamma^{(k)}_{ijklk_1..k_k}(\underline{x}_{\gamma\alpha}) [W_0^{r+k-i,0}(\Omega'_\alpha)]_{k_1..k_{k-i} r_1..r_r} [W_0^{i+s,0}(\Omega'_\gamma)]_{k_{k-i+1}..k_k s_1..s_s}$$

$$\left. \begin{array}{l} {}^n\Gamma_{ijkl}(\underline{x} - \underline{y} + \underline{x}_{\gamma\alpha}) = {}^n\Gamma_{klij}(\underline{y} - \underline{x} + \underline{x}_{\alpha\gamma}) \\ {}^n\Gamma_{ijkl}(\underline{x} - \underline{y} + \underline{x}_{\gamma\alpha}) = {}^n\Gamma_{klij}(\underline{x} - \underline{y} + \underline{x}_{\gamma\alpha}) \end{array} \right| \begin{array}{l} \Longrightarrow ({}^n T^{\alpha\gamma}_{r,s})_{r_1 \ldots r_r klij s_1 \ldots s_s} = ({}^n T^{\alpha\gamma}_{r,s})_{r_1 \ldots r_r ijkl s_1 \ldots s_s} \\ \Longrightarrow ({}^n T^{\gamma\alpha}_{s,r})_{s_1 \ldots s_s klij r_1 \ldots r_r} = ({}^n T^{\alpha\gamma}_{r,s})_{r_1 \ldots r_r ijkl s_1 \ldots s_s} \end{array}$$

Self-influence tensors for polarization fields in $\mathcal{V}^{h_p}$

Similarly as before, we want to address the terms with those components:

$$\int_{\Omega_\alpha}\int_{\Omega_\alpha}(x_{r_1}-x^\alpha_{r_1})\ldots(x_{r_r}-x^\alpha_{r_r})\Gamma_{ijkl}(\underline{x}-\underline{y})(y_{s_1}-x^\alpha_{s_1})\ldots(y_{s_s}-x^\alpha_{s_s})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}}$$

$$=$$

Change of variable

$$\int_{\Omega^\gamma_\alpha}\int_{\Omega'_\alpha}x_{r_1}\ldots x_{r_r}\Gamma_{ijkl}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})(y_{s_1}-x^{\gamma\alpha}_{s_1})\ldots(y_{s_s}-x^{\gamma\alpha}_{s_s})\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}}$$

$$\Omega'_\alpha := \Omega_\alpha \uplus \{-\underline{x}_\alpha\}$$
$$\Omega^\gamma_\alpha := \Omega_\alpha \uplus \{-\underline{x}_\gamma\}$$
$$= \Omega'_\alpha \uplus \{\underline{x}_{\gamma\alpha}\}$$

so that the following estimates of the "*r-s* self-influence tensor of Ω_α" are obtained after picking some $\gamma \neq \alpha$,

$$({}^nT^{\alpha\alpha}_{r,s})_{r_1\ldots r_r ijkl s_1\ldots s_s} = \frac{1}{|\Omega|}[W_0^{r,0}(\Omega'_\alpha)]_{r_1\ldots r_r}\Gamma_{ijkl}(\underline{x}_{\gamma\alpha})[W_0^{s,0}(\Omega'_\alpha)]_{s_1\ldots s_s}$$

for any $\gamma \neq \alpha$

$$+\frac{1}{|\Omega|}\sum_{k=1}^{n}\sum_{i=0}^{k}\frac{(-1)^i}{(k-i)!i!}\Gamma^{(k)}_{ijklk_1..k_k}(\underline{x}_{\gamma\alpha})[W_0^{r+k-i,0}(\Omega'_\alpha)]_{k_1..k_{k-i}r_1..r_r}[{}^\gamma\widetilde{\mathcal{W}}_0^{i|s,0}(\Omega'_\alpha)]_{k_{k-i+1}\ldots k_k s_1\ldots s_s}$$

where

$${}^\gamma\widetilde{\mathcal{W}}_0^{i|s,0}(\Omega'_\alpha) := \sum_{t=0}^{i}\binom{i}{t}(\underline{x}_{\gamma\alpha})^{\otimes^{i-t}} \overset{i-t,t}{\odot} \mathcal{W}_0^{t+s,0}(\Omega'_\alpha)$$

Which, once again, can be obtained by post-processing the Minkowski tensors computed previously.

HS functional for trial fields in $\mathcal{V}^{h_p}$ (derivation)

From our definition of the estimates of influence tensors, we obtain

$$\overline{\boldsymbol{\tau}^{h_p} : {}^{n}(\boldsymbol{\Gamma} * \boldsymbol{\tau}^{h_p})} = \sum_{\alpha}\sum_{\gamma}\left[\boldsymbol{\tau}^{\alpha} : {}^{n}\mathbb{T}^{\alpha\gamma}_{0,0} : \boldsymbol{\tau}^{\gamma} + \sum_{r=1}^{p}\sum_{s=1}^{p}\left\langle \boldsymbol{\partial}^{r}\boldsymbol{\tau}^{\alpha}, \left\langle {}^{n}\mathbb{T}^{\alpha\gamma}_{r,s}, \boldsymbol{\tau}^{\gamma}\boldsymbol{\partial}^{s}\right\rangle_{s+2}\right\rangle_{r+2}\right]$$

The other term, $\overline{\boldsymbol{\tau}^{h_p} : (\Delta\mathbb{L})^{-1} : \boldsymbol{\tau}^{h_p}}$ can be calculated exactly. We obtain

$$\overline{\boldsymbol{\tau}^{h_p} : (\Delta\mathbb{L})^{-1} : \boldsymbol{\tau}^{h_p}} = \sum_{\alpha}\Delta\mathbb{M}^{\alpha} :: \left[c_{\alpha}\boldsymbol{\tau}^{\alpha}\otimes\boldsymbol{\tau}^{\alpha} + \sum_{r=1}^{p}\sum_{s=1}^{p}\left\langle \boldsymbol{\tau}^{\alpha}\boldsymbol{\partial}^{r}, \left\langle \mathcal{W}_{0}^{r+s,0}(\Omega'_{\alpha}), \boldsymbol{\partial}^{s}\boldsymbol{\tau}^{\alpha}\right\rangle_{s}\right\rangle_{r}\right]$$

where $\Delta\mathbb{M}^{\alpha} := (\mathbb{L}^{\alpha} - \mathbb{L}^{0})^{-1}$ so that the following estimate of the HS functional ${}^{n}\mathcal{H}(\boldsymbol{\tau}^{h_p}) := \overline{\boldsymbol{\tau}^{h_p}} : \overline{\boldsymbol{\varepsilon}} - 1/2\overline{\boldsymbol{\tau}^{h_p} : (\Delta\mathbb{L})^{-1} : \boldsymbol{\tau}^{h_p}} - 1/2\overline{\boldsymbol{\tau}^{h_p} : {}^{n}(\boldsymbol{\Gamma} * \boldsymbol{\tau}^{h_p})}$ is

$$\begin{aligned}
{}^{n}\mathcal{H}(\boldsymbol{\tau}^{h_p}) = \sum_{\alpha}&\left(c_{\alpha}\boldsymbol{\tau}^{\alpha} : \overline{\boldsymbol{\varepsilon}} + \sum_{r=1}^{p}\left\langle \boldsymbol{\tau}^{\alpha}\boldsymbol{\partial}^{r}, \mathcal{W}_{0}^{r,0}(\Omega'_{\alpha})\right\rangle_{r} : \overline{\boldsymbol{\varepsilon}}\right) \\
&-\frac{1}{2}\sum_{\alpha}\Delta\mathbb{M}^{\alpha} :: \left(c_{\alpha}\boldsymbol{\tau}^{\alpha}\otimes\boldsymbol{\tau}^{\alpha} + \sum_{r=1}^{p}\sum_{s=1}^{p}\left\langle \boldsymbol{\tau}^{\alpha}\boldsymbol{\partial}^{r}, \left\langle \mathcal{W}_{0}^{r+s,0}(\Omega'_{\alpha}), \boldsymbol{\partial}^{s}\boldsymbol{\tau}^{\alpha}\right\rangle_{s}\right\rangle_{r}\right) \\
&-\frac{1}{2}\sum_{\alpha}\sum_{\gamma}\left(\boldsymbol{\tau}^{\alpha} : {}^{n}\mathbb{T}^{\alpha\gamma}_{0,0} : \boldsymbol{\tau}^{\gamma} + \sum_{r=1}^{p}\sum_{s=1}^{p}\left\langle \boldsymbol{\partial}^{r}\boldsymbol{\tau}^{\alpha}, \left\langle {}^{n}\mathbb{T}^{\alpha\gamma}_{r,s}, \boldsymbol{\tau}^{\gamma}\boldsymbol{\partial}^{s}\right\rangle_{s+2}\right\rangle_{r+2}\right)
\end{aligned}$$

Stationarity conditions for trial fields in $\mathcal{V}^{h_p}$

The stationary state of the functional is such that

First, let $\boldsymbol{\partial}_{\boldsymbol{\tau}^\alpha}{}^n\mathcal{H} = \mathbf{0}$ for all α :

After using $({}^nT_{0,0}^{\gamma\alpha})_{ijkl} = ({}^nT_{0,0}^{\alpha\gamma})_{klij}$ for $\gamma \neq \alpha$ and symmetrizing our estimates of self-influence tensors ${}^n\mathbb{T}_{0,0}^{\alpha\alpha}$, we obtain

$$c_\alpha \overline{\boldsymbol{\varepsilon}} = c_\alpha \Delta\mathbb{M}^\alpha : \boldsymbol{\tau}^\alpha + \sum_\gamma {}^n\mathbb{T}_{0,0}^{\alpha\gamma} : \boldsymbol{\tau}^\gamma \quad \text{for all } \alpha.$$

Second, let $\boldsymbol{\partial}_{\boldsymbol{\tau}^\alpha \boldsymbol{\partial}^r}{}^n\mathcal{H} = \mathbf{0}$ for all α, r s.t. $1 \leq r \leq p$:

Similarly, after using $({}^nT_{0,0}^{\gamma\alpha})_{r_1 \dots r_r ijkl s_1 \dots s_s} = ({}^nT_{0,0}^{\alpha\gamma})_{s_1 \dots s_s klij r_1 \dots r_r}$ for $\gamma \neq \alpha$ and symmetrizing our estimates of self-influence tensors ${}^n\mathbb{T}_{s,r}^{\alpha\alpha}$, we obtain

$$\overline{\boldsymbol{\varepsilon}} \otimes \mathcal{W}_0^{r,0}(\Omega'_\alpha) = \Delta\mathbb{M}^\alpha : \sum_{s=1}^{p} \left\langle \boldsymbol{\tau}^\alpha \boldsymbol{\partial}^s, \mathcal{W}_0^{s+r,0}(\Omega'_\alpha) \right\rangle_s + \sum_\gamma \sum_{s=1}^{p} \left\langle \boldsymbol{\partial}^s \boldsymbol{\tau}^\gamma, {}^n\mathbb{T}_{s,r}^{\gamma\alpha} \right\rangle_{s+2}$$

for all α, r s.t. $1 \leq r \leq p$:

"Generalized Mandel representation" for assembly of a global system of stationarity equations

We want to solve the system

$$r=0 \quad \rightarrow \underset{3n_\alpha\times 1}{\{\overline{\boldsymbol{\varepsilon}}^0\}} = \underset{3n_\alpha\times 3n_\alpha}{[\mathbb{D}^0_0]}\underset{3n_\alpha\times 1}{\{\boldsymbol{\tau}\}}$$

$$r=1 \quad \rightarrow \underset{6n_\alpha\times 1}{\{\overline{\boldsymbol{\varepsilon}}^1\}} = \underset{6n_\alpha\times 6n_\alpha}{[\mathbb{D}^1_1]}\underset{6n_\alpha\times 1}{\{\boldsymbol{\partial\tau}\}} + \underset{6n_\alpha\times 9n_\alpha}{[\mathbb{D}^1_2]}\underset{9n_\alpha\times 1}{\{\boldsymbol{\partial}^2\boldsymbol{\tau}\}} + \underset{6n_\alpha\times 12n_\alpha}{[\mathbb{D}^1_3]}\underset{12n_\alpha\times 1}{\{\boldsymbol{\partial}^3\boldsymbol{\tau}\}} + \cdots + \underset{6n_\alpha\times 3(p+1)n_\alpha}{[\mathbb{D}^1_p]}\overset{3(p+1)n_\alpha\times 1}{\{\boldsymbol{\partial}^p\boldsymbol{\tau}\}}$$

$$r=2 \quad \rightarrow \underset{9n_\alpha\times 1}{\{\overline{\boldsymbol{\varepsilon}}^2\}} = \underset{9n_\alpha\times 6n_\alpha}{[\mathbb{D}^2_1]}\underset{6n_\alpha\times 1}{\{\boldsymbol{\partial\tau}\}} + \underset{9n_\alpha\times 9n_\alpha}{[\mathbb{D}^2_2]}\underset{9n_\alpha\times 1}{\{\boldsymbol{\partial}^2\boldsymbol{\tau}\}} + \underset{9n_\alpha\times 12n_\alpha}{[\mathbb{D}^2_3]}\underset{12n_\alpha\times 1}{\{\boldsymbol{\partial}^3\boldsymbol{\tau}\}} + \cdots + \underset{9n_\alpha\times 3(p+1)n_\alpha}{[\mathbb{D}^2_p]}\overset{3(p+1)n_\alpha\times 1}{\{\boldsymbol{\partial}^p\boldsymbol{\tau}\}}$$

$$r=3 \quad \rightarrow \underset{12n_\alpha\times 1}{\{\overline{\boldsymbol{\varepsilon}}^3\}} = \underset{12n_\alpha\times 6n_\alpha}{[\mathbb{D}^3_1]}\underset{6n_\alpha\times 1}{\{\boldsymbol{\partial\tau}\}} + \underset{12n_\alpha\times 9n_\alpha}{[\mathbb{D}^3_2]}\underset{9n_\alpha\times 1}{\{\boldsymbol{\partial}^2\boldsymbol{\tau}\}} + \underset{12n_\alpha\times 12n_\alpha}{[\mathbb{D}^3_3]}\underset{12n_\alpha\times 1}{\{\boldsymbol{\partial}^3\boldsymbol{\tau}\}} + \cdots + \underset{12n_\alpha\times 3(p+1)n_\alpha}{[\mathbb{D}^3_p]}\overset{3(p+1)n_\alpha\times 1}{\{\boldsymbol{\partial}^p\boldsymbol{\tau}\}}$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad \ddots \qquad \vdots$$

$$r=p \quad \rightarrow \underset{3(p+1)n_\alpha\times 1}{\{\overline{\boldsymbol{\varepsilon}}^p\}} = \underset{3(p+1)n_\alpha\times 6n_\alpha}{[\mathbb{D}^p_1]}\overset{6n_\alpha\times 1}{\{\boldsymbol{\partial\tau}\}} + \underset{3(p+1)n_\alpha\times 9n_\alpha}{[\mathbb{D}^p_2]}\overset{9n_\alpha\times 1}{\{\boldsymbol{\partial}^2\boldsymbol{\tau}\}} + \underset{3(p+1)n_\alpha\times 12n_\alpha}{[\mathbb{D}^p_3]}\overset{12n_\alpha\times 1}{\{\boldsymbol{\partial}^3\boldsymbol{\tau}\}} + \cdots + \underset{3(p+1)n_\alpha\times 3(p+1)n_\alpha}{[\mathbb{D}^p_p]}\overset{3(p+1)n_\alpha\times 1}{\{\boldsymbol{\partial}^p\boldsymbol{\tau}\}}$$

which we recast in

$$\underset{\frac{3n_\alpha}{2}(p^2+3p)\times 1}{\begin{Bmatrix} \{\overline{\boldsymbol{\varepsilon}}^1\} \\ \{\overline{\boldsymbol{\varepsilon}}^2\} \\ \{\overline{\boldsymbol{\varepsilon}}^2\} \\ \vdots \\ \{\overline{\boldsymbol{\varepsilon}}^p\} \end{Bmatrix}} = \underset{\frac{3n_\alpha}{2}(p^2+3p)\times\frac{3n_\alpha}{2}(p^2+3p)}{\begin{bmatrix} [\mathbb{D}^1_1] & [\mathbb{D}^1_2] & [\mathbb{D}^1_3] & \dots & [\mathbb{D}^1_p] \\ [\mathbb{D}^2_1] & [\mathbb{D}^2_2] & [\mathbb{D}^2_3] & \dots & [\mathbb{D}^2_p] \\ [\mathbb{D}^3_1] & [\mathbb{D}^3_2] & [\mathbb{D}^3_3] & \dots & [\mathbb{D}^3_p] \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ [\mathbb{D}^p_1] & [\mathbb{D}^p_2] & [\mathbb{D}^p_3] & \dots & [\mathbb{D}^p_p] \end{bmatrix}} \underset{\frac{3n_\alpha}{2}(p^2+3p)\times 1}{\begin{Bmatrix} \{\boldsymbol{\partial\tau}\} \\ \{\boldsymbol{\partial}^2\boldsymbol{\tau}\} \\ \{\boldsymbol{\partial}^3\boldsymbol{\tau}\} \\ \vdots \\ \{\boldsymbol{\partial}^p\boldsymbol{\tau}\} \end{Bmatrix}}$$

where

$$[\mathbb{D}^r_s] := [\mathbb{M}_{s,r}] + [\mathbb{T}_{s,r}]$$

- $[\mathbb{M}_{s,r}]$: Assembly of components of compliances $\Delta\mathbb{M}^\alpha$ weighted by Minkowski tensors.
- $[\mathbb{T}_{s,r}]$: Assembly of components of self-influence and influence tensors.

Computation of a table of derivatives of Green operators

- For some given order *n* of the Taylor expansion used for the Green operators, we need to compute

$$\Gamma_{ijkl,k_1}(\underline{x}_{\gamma\alpha}),\ \Gamma^{(1)}_{ijkl,k_1}(\underline{x}_{\gamma\alpha}),\ \Gamma^{(2)}_{ijkl,k_1k_2}(\underline{x}_{\gamma\alpha}),\ \ldots,\Gamma^{(n)}_{ijkl,k_1\ldots k_k}(\underline{x}_{\gamma\alpha})$$

- Taking advantage of symmetries, if all pairwise interactions are to be accounted for, this means that

$$6\binom{n_\alpha}{2}\binom{n+2}{2} = \frac{3(n_\alpha-1)n_\alpha(n+1)(n+2)}{2}$$

components need to be evaluated.

- The construction of the table of derivatives is what governs the computing time of the current implementation.

- In a later time, it would be relevant to introduce "*k-fold neighborhoods*" by limiting the number of grains Ω_γ interacting with a grain Ω_α to the $\tilde{n}_\alpha(\alpha,1)<n_\alpha$ nearest neighbors, or to the $\tilde{n}_\alpha(\alpha,2)<n_\alpha$ first and second nearest neighbors, and so on...

2D Barnett-Lothe integral formalism

- The Green operator obtained as follows from the Green's function,

$$4\Gamma_{ijkl}(r,\theta) := G^{(2)}_{ik,jl}(r,\theta) + G^{(2)}_{il,jk}(r,\theta) + G^{(2)}_{jk,il}(r,\theta) + G^{(2)}_{jl,ik}(r,\theta)$$

- Irrespectively of the material symmetry, 2D Green's functions are a by-product of the Barnett-Lothe (1973) integral formalism. We have

$$2\mathbf{G}(r,\theta) = -\frac{1}{\pi}\ln(r)\mathbf{H}(\pi) - \mathbf{S}(\theta)\cdot\mathbf{H}(\pi) - \mathbf{H}(\theta)\cdot\mathbf{S}^T(\pi)$$

  where $\mathbf{S}(\theta) = \frac{1}{\pi}\int_0^\theta \mathbf{N}^1(\psi)\mathrm{d}\psi$ and $\mathbf{H}(\theta) = \frac{1}{\pi}\int_0^\theta \mathbf{N}^2(\psi)\mathrm{d}\psi$ are incomplete Barnett-Lothe integrals with integrands readily computable for every symmetry.

- To evaluate Γ_{ijkl}, we only need those integrands and the complete integrals $\mathbf{S}(\pi)$ and $\mathbf{H}(\pi)$, which we evaluate numerically.
- We derive the following recurrence relations:

$$2\pi G^{(n)}_{ij,k_1\ldots k_n}(r,\theta) = (-r)^{-n} h^n_{ijk_1\ldots k_n}(\theta)$$

$$h^n_{ijk_1\ldots k_n}(\theta) = (n-1)h^{n-1}_{ijk_1\ldots k_{n-1}}(\theta)n_{k_n}(\theta) - \partial_\theta[h^{n-1}_{ijk_1\ldots k_{n-1}}(\theta)]m_{k_n}(\theta) \quad \text{for } n\geq 2$$

Requires evaluation of $\partial^k_\theta[N^1_{il}(\theta)]$ and $\partial^k_\theta[N^2_{il}(\theta)]$ for $k=0,\ldots,n-1$

$$\partial^k_\theta[h^n_{ijk_1\ldots k_n}(\theta)] = \sum_{s=0}^{k}\binom{k}{s}\left\{(n-1)\partial^{k-s}_\theta[h^{n-1}_{ijk_1\ldots k_{n-1}}(\theta)]\partial^s_\theta[n_{k_n}(\theta)] - \partial^{k-s+1}_\theta[h^{n-1}_{ijk_1\ldots k_{n-1}}(\theta)]\partial^{s+1}_\theta[n_{k_n}(\theta)]\right\}$$

$$h^1_{ijk_1}(\theta) = H_{ij}n_{k_1}(\theta) + [N^1_{is}(\theta)H_{sj} + N^2_{is}(\theta)S_{js}]m_{k_1}(\theta)$$

$$\partial^k_\theta[h^1_{ijk_1}(\theta)] = H_{ij}\partial^k_\theta[n_{k_1}(\theta)] + \sum_{s=0}^{k}\binom{k}{s}\left\{H_{lj}\partial^{k-s}_\theta[N^1_{il}(\theta)] + S_{jl}\partial^{k-s}_\theta[N^2_{il}(\theta)]\right\}\partial^s_\theta[m_{k_1}(\theta)]$$

2D Anisotropy

- Polar representation of 2D anisotropic stiffnesses, see Vannucci (2016)

$$L_{1111} = T_0 + 2T_1 + R_0\cos(4\Phi_0) + 4R_1\cos(2\Phi_1)$$
$$L_{1112} = R_0\sin(4\Phi_0) + 2R_1\sin(2\Phi_1)$$
$$L_{1122} = -T_0 + 2T_1 - R_0\cos(4\Phi_0)$$
$$L_{1212} = T_0 - R_0\cos(4\Phi_0)$$
$$L_{2212} = -R_0\sin(4\Phi_0) + 2R_1\sin(2\Phi_1)$$
$$L_{2222} = T_0 + 2T_1 + R_0\cos(4\Phi_0) - 4R_1\cos(2\Phi_1)$$

$$T_0,\ T_1 : \text{Isotropic polar invariants}$$
$$R_0,\ R_1,\ \Phi_0 - \Phi_1 : \text{Anisotropic polar invariants}$$

Substitute Φ_j by $\Phi_j - \theta$ for counter clockwise positive passive rotation

Conditions for positive strain energy

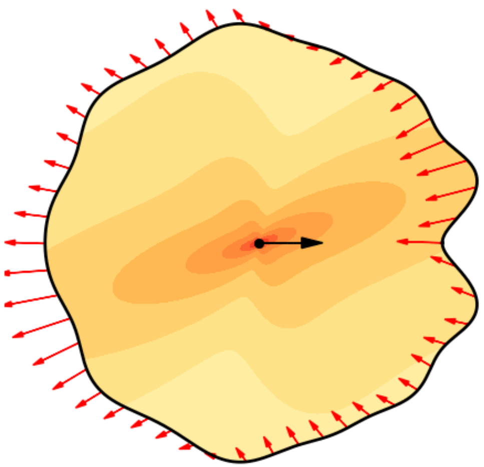
$$T_0 - R_0 > 0,$$
$$T_1(T_0^2 - R_0^2) - 2R_1^2\{T_0 - R_0\cos[4(\Phi_0 - \Phi_1)]\} > 0,$$
$$R_0 \geq 0,$$
$$R_1 \geq 0.$$

$$R_0R_1^2\sin[4(\Phi_0 - \Phi_1)] \neq 0$$

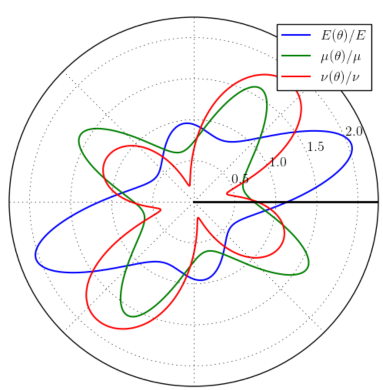
$$R_0R_1^2\sin[4(\Phi_0 - \Phi_1)] = 0 \implies \text{Symmetry}$$

Validation

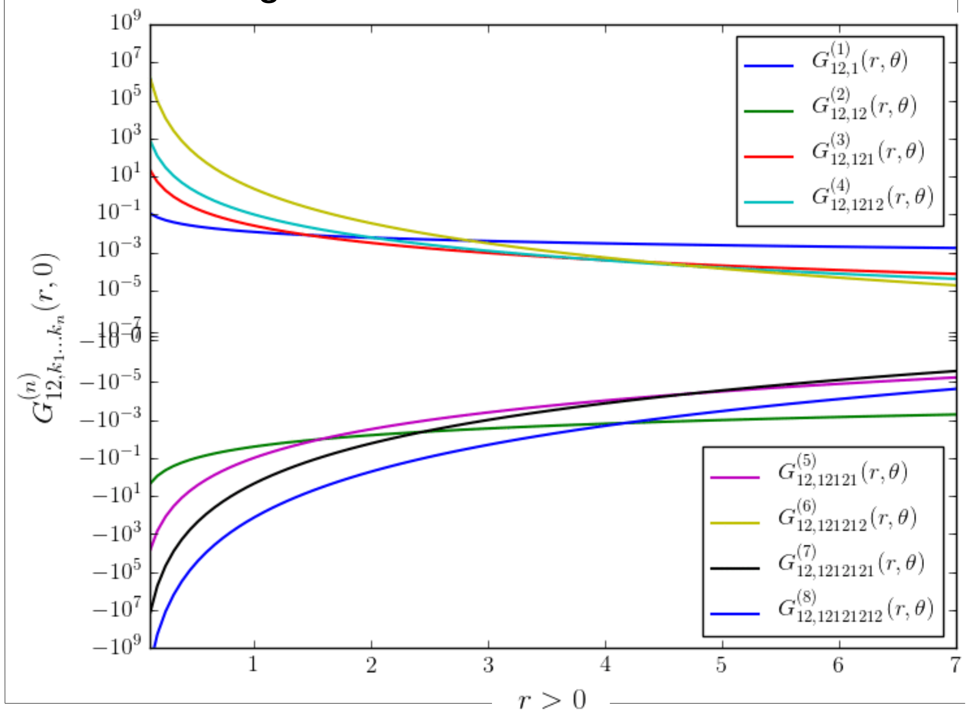
Equilibrated traction fields on random curves



Polar diagram of generalized moduli



Computed components of some gradients of the Green's function



Morphological characterization for simple geometries

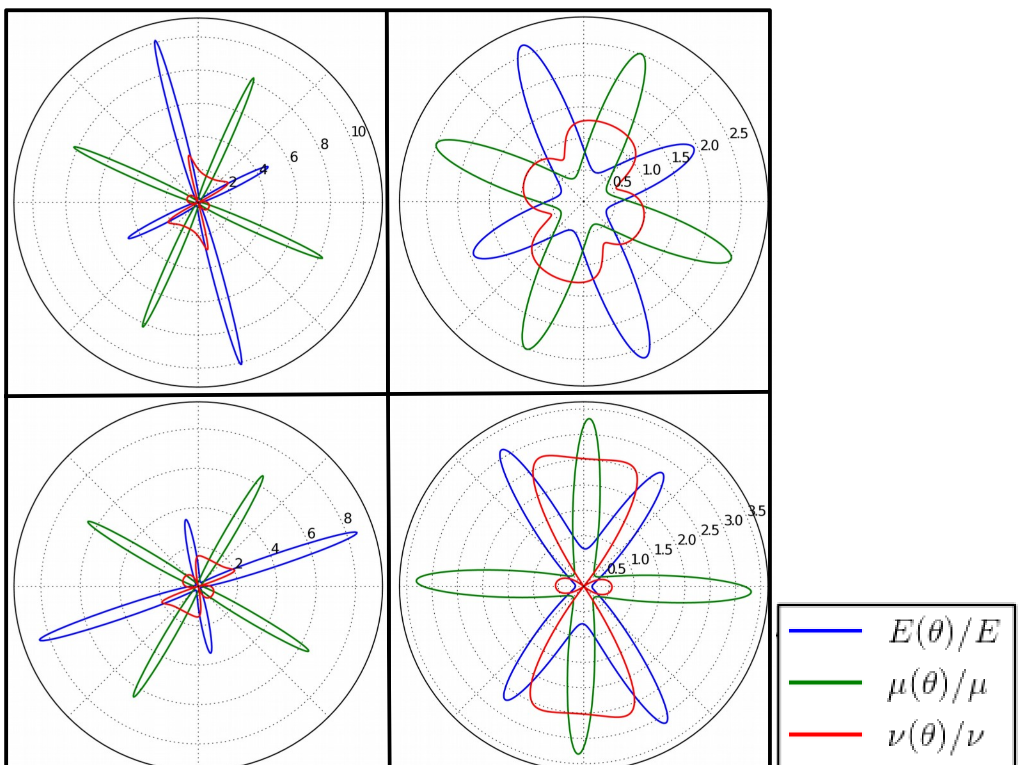
- As a first application, we consider a 2D periodic array of anisotropic squares. The corresponding Minkowski tensors of interest have components

$$[\mathcal{W}_0^{r,0}](n_1) := [\mathcal{W}_0^{r,0}]_{\underbrace{11\ldots1}_{(n_1 \text{ times})}\underbrace{22\ldots2}_{(r-n_1 \text{ times})}}$$

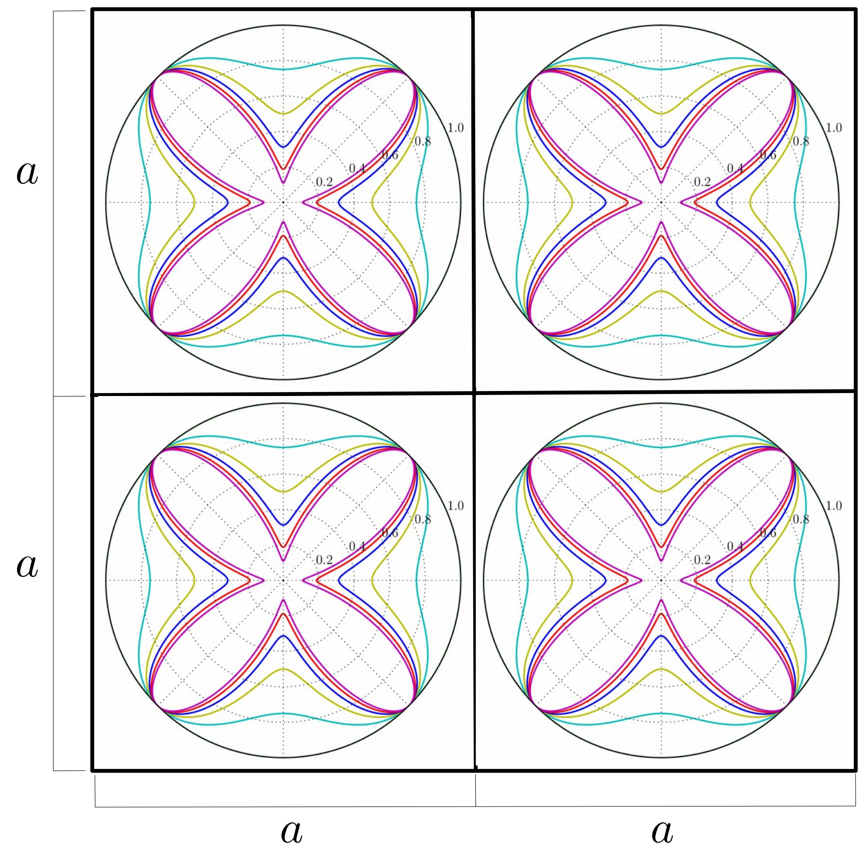
$$n_1 \in [0, r]$$
$$n_2 := r - n_1$$

$$[\mathcal{W}_0^{r,0}](n_1) = \frac{(a/2)^{n_1+n_2+2} - (-a/2)^{n_1+1}(a/2)^{n_2+1} - (a/2)^{n_1+1}(-a/2)^{n_2+1} + (-a/2)^{n_1+1}(-a/2)^{n_2+1}}{(n_1+1)(n_2+1)}$$

Polar diagram of generalized moduli



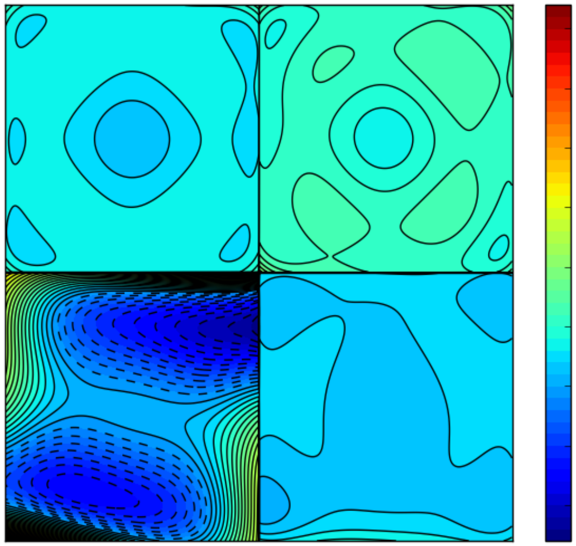
Reynolds glyphs of normalized Minkowski tensors $\mathcal{W}_0^{r,0}$ for $r \leq 12$



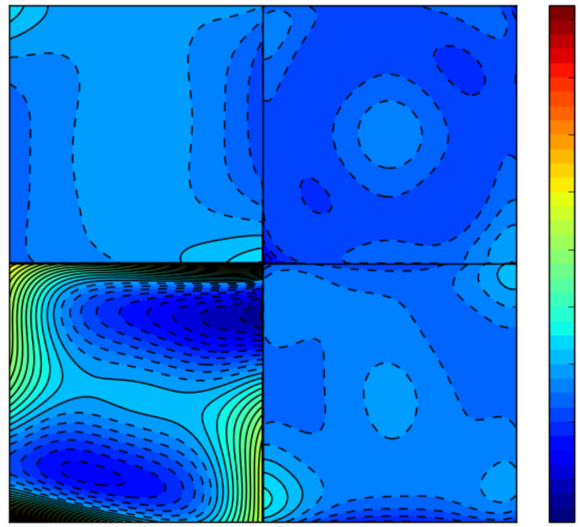
Results

- Preliminary results for a uniaxial average strain $\langle \boldsymbol{\varepsilon} \rangle = \underline{e}_2 \otimes \underline{e}_2$

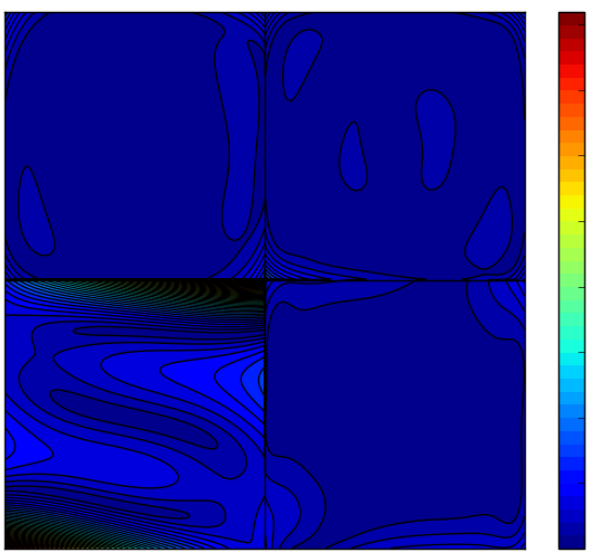
$(\tau_{11}/T_0)(T_0 + T_1)/(T_0 + 2T_1)$



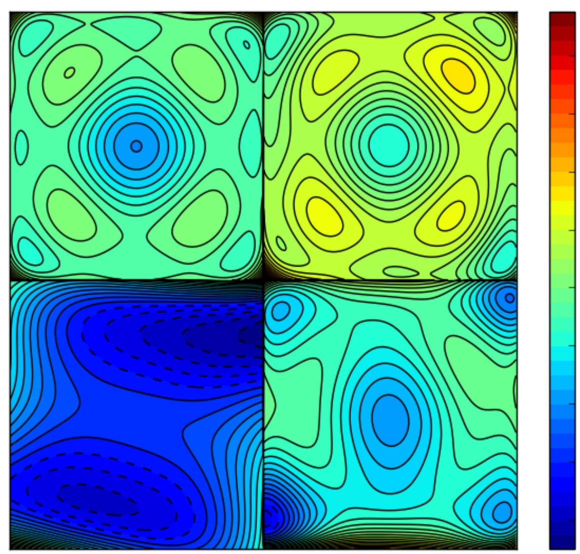
τ_{12}/T_0



$\|\nabla \cdot \boldsymbol{\tau}\|$



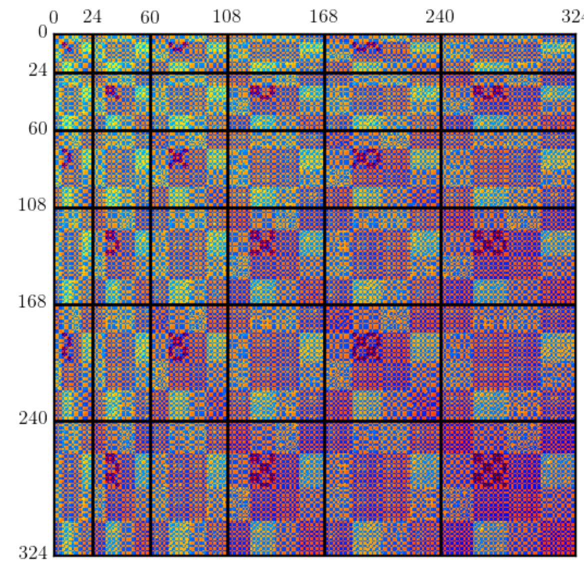
$(\tau_{22}/T_0)(T_0 + T_1)/(T_0 + 2T_1)$



Note that

$$\begin{bmatrix} [\mathbb{D}_1^1] & [\mathbb{D}_2^1] & [\mathbb{D}_3^1] & \cdots & [\mathbb{D}_p^1] \\ [\mathbb{D}_1^2] & [\mathbb{D}_2^2] & [\mathbb{D}_3^2] & \cdots & [\mathbb{D}_p^2] \\ [\mathbb{D}_1^3] & [\mathbb{D}_2^3] & [\mathbb{D}_3^3] & \cdots & [\mathbb{D}_p^3] \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ [\mathbb{D}_1^p] & [\mathbb{D}_2^p] & [\mathbb{D}_3^p] & \cdots & [\mathbb{D}_p^p] \end{bmatrix}$$

is symmetric because Ω'_α has the same morphology for all α



Post-processing

- Once an estimate of the polarization stress field is obtained, there are different ways to obtain the corresponding strain field

  – First, from the very definition of the polarization, we have

$$\boldsymbol{\varepsilon}(\underline{x}) = \Delta\mathbb{M}(\underline{x}) : \boldsymbol{\tau}(\underline{x})$$

  If so, we can recover closed form expressions of the corresponding piecewise polynomial strain and strain fields:

$$\boldsymbol{\varepsilon}^{h_p}(\underline{x}) = \sum_{\alpha} \left(\chi_\alpha(\underline{x})\boldsymbol{\varepsilon}^{\alpha} + \chi_\alpha(\underline{x}) \sum_{k=1}^{p} \left\langle \boldsymbol{\varepsilon}^{\alpha}\boldsymbol{\partial}^{k}, (\underline{x} - \underline{x}^{\alpha})^{\otimes^k} \right\rangle_k \right)$$

and $$\boldsymbol{\sigma}^{h_p}(\underline{x}) = \sum_{\alpha} \left(\chi_\alpha(\underline{x})\boldsymbol{\sigma}^{\alpha} + \chi_\alpha(\underline{x}) \sum_{k=1}^{p} \left\langle \boldsymbol{\sigma}^{\alpha}\boldsymbol{\partial}^{k}, (\underline{x} - \underline{x}^{\alpha})^{\otimes^k} \right\rangle_k \right)$$

  However, as we do so, we note that *the “prescribed” mean strain state is not recovered*.

  – Another possibility is to exploit the following form of the Lippman-Schwinger equation

$$\boldsymbol{\varepsilon}(\underline{x}) = \overline{\boldsymbol{\varepsilon}} - {}^{n}\boldsymbol{\Gamma} * \boldsymbol{\tau}^{h_p}(\underline{x})$$

  for which derivations as the ones carried over for the definition of the influence tensors is needed.

Post-processing

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  - First, from the very definition of the polarization, we have

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$$\boldsymbol{\varepsilon}^{h_p}(\underline{x}) = \sum_{\alpha} \left(\chi_\alpha(\underline{x}) \boldsymbol{\varepsilon}^{\alpha} + \chi_\alpha(\underline{x}) \sum_{k=1}^{p} \left\langle \boldsymbol{\varepsilon}^{\alpha} \boldsymbol{\partial}^{k}, (\underline{x} - \underline{x}^{\alpha})^{\otimes^k} \right\rangle_k \right)$$

and $$\boldsymbol{\sigma}^{h_p}(\underline{x}) = \sum_{\alpha} \left(\chi_\alpha(\underline{x}) \boldsymbol{\sigma}^{\alpha} + \chi_\alpha(\underline{x}) \sum_{k=1}^{p} \left\langle \boldsymbol{\sigma}^{\alpha} \boldsymbol{\partial}^{k}, (\underline{x} - \underline{x}^{\alpha})^{\otimes^k} \right\rangle_k \right)$$

However, as we do so, we note that <u>*the "prescribed" mean strain state is not recovered*</u>.

  - Another possibility is to exploit the following form of the Lippman-Schwinger equation

$$\boldsymbol{\varepsilon}(\underline{x}) = \overline{\boldsymbol{\varepsilon}} - {}^{n}\boldsymbol{\Gamma} * \boldsymbol{\tau}^{h_p}$$

Work in progress

for which derivations as the ones carried on of the influence tensors is needed.

References

- **Barnett, D. and Lothe, J.** (1973). Synthesis of the sextic and the integral formalism for dislocations, greens functions and surface waves in anisotropic elastic solids. *Phys. Norv.*, 7:13–19.
- **Brisard, S.** (2011). Analyse morphologique et homogénéisation numérique: application á la pâte de ciment. PhD thesis, *Université Paris-Est*.
- **Brisard, S., Dormieux, L., and Sab, K.** (2014). A variational form of the equivalent inclusion method for numerical homogenization. *International Journal of Solids and Structures, 51(3):716 – 728.*
- **Eshelby, J., Read, W., and Shockley, W.** (1953). Anisotropic elasticity with applications to dislocation theory. *Acta Metallurgica*, 1(3):251–259.
- **Hashin, Z. and Shtrikman, S.** (1962). On some variational principles in anisotropic and nonhomogeneous elasticity. *Journal of the Mechanics and Physics of Solids*, 10(4):335–342.
- **Molinari, A.** (2001). Averaging models for heterogeneous viscoplastic and elastic viscoplastic materials. *Journal of Engineering Materials and Technology*, 124(1):62–70.
- **Ponte-Castaneda, P. and Willis, J.** (1995). The effect of spatial distribution on the effective behavior of composite materials and cracked media. *Journal of the Mechanics and Physics of Solids*, 43(12):1919–1951.
- **Stroh, A. N.** (1958). Dislocations and cracks in anisotropic elasticity. *Philosophical Magazine*, 3(30):625–646.
- **Stroh, A. N.** (1962). Steady state problems in anisotropic elasticity. *Journal of Mathematics and Physics*, 41(1-4):77–103.
- **Ting, T.** (1996). Anisotropic Elasticity: Theory and Applications. *Oxford University Press*.
- **Torquato, S.** (1997). Effective stiffness tensor of composite mediai. exact series expansions. *Journal of the Mechanics and Physics of Solids*, 45(9):1421–1448.
- **Vannucci, P.** (2016). Another View on Planar Anisotropy: The Polar Formalism, pages 489–524. *Springer International Publishing, Cham.*
- **Willis, J.** (1977). Bounds and self-consistent estimates for the overall properties of anisotropic composites. *Journal of the Mechanics and Physics of Solids*, 25(3):185–202.