Effect of Morphological Idealization on Mean-Field Self-Consistent Homogenization of Polycrystals

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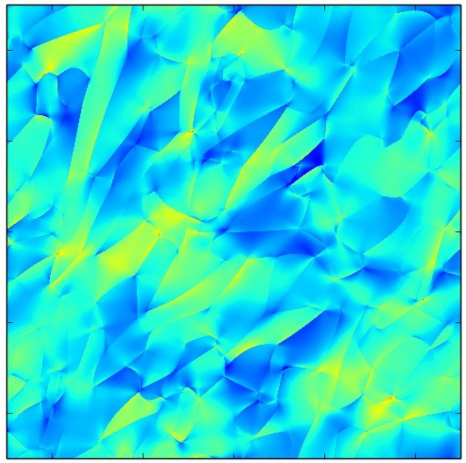
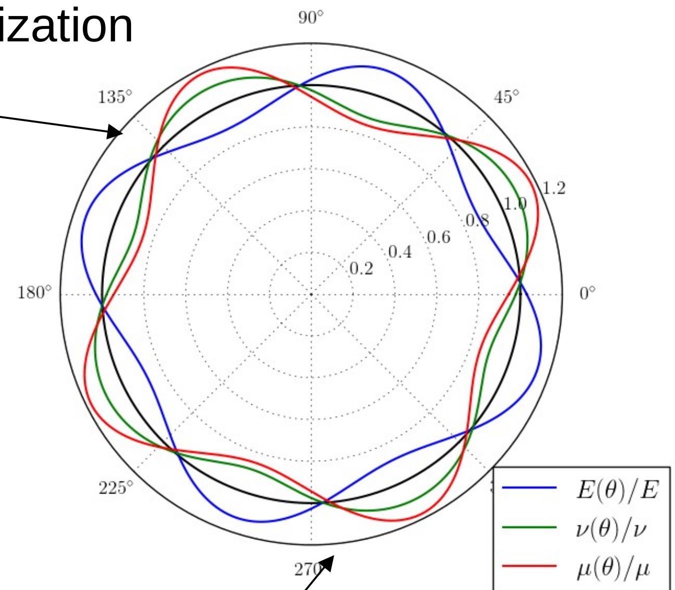
Motivation and objective

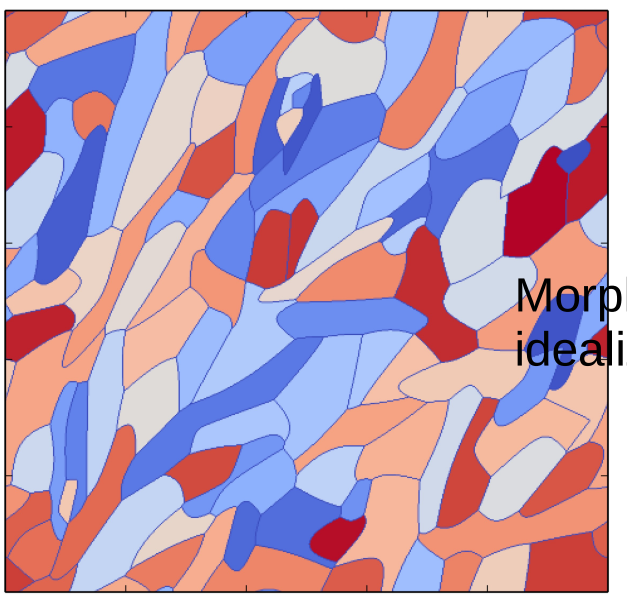
- Identify best idealization

Numerical homogenization

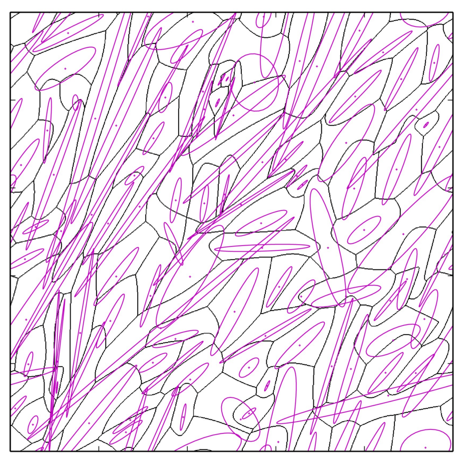




Full-field simulation



Morphology idealization



Mean-field self-consistent homogenization

Outline

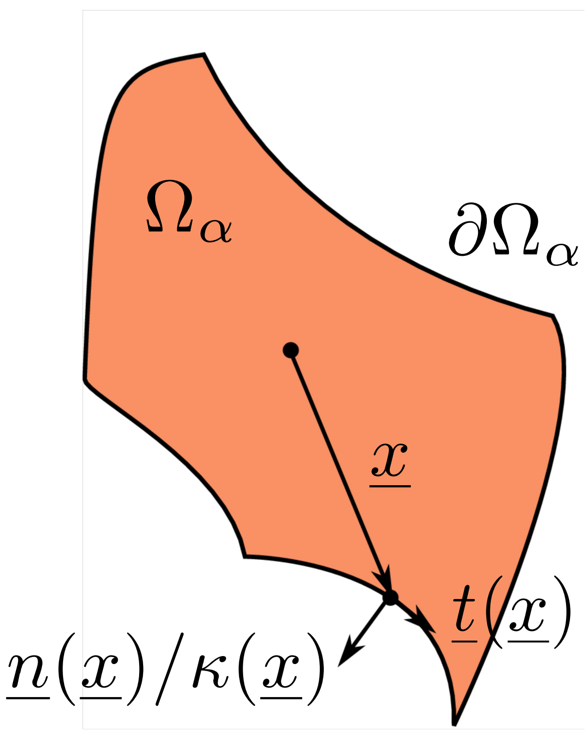
- Morphological characterization of single grains
- Numerical homogenization
- Self-consistent homogenization
- Shape idealization
- Comparison of SC estimates of elastic stiffness

Single grain morphology characterization

Single grains are characterized using Minkowski tensors:

Measures of mass distribution:

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

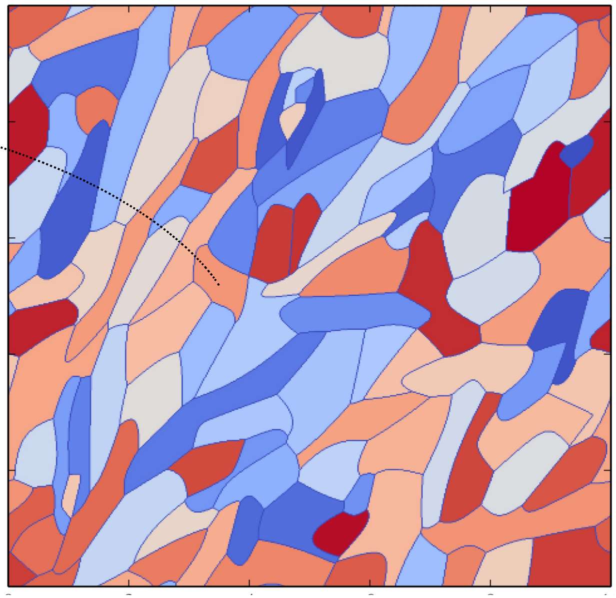


Measures of surface distribution:

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

Curvature-weighted measures of surface distribution:

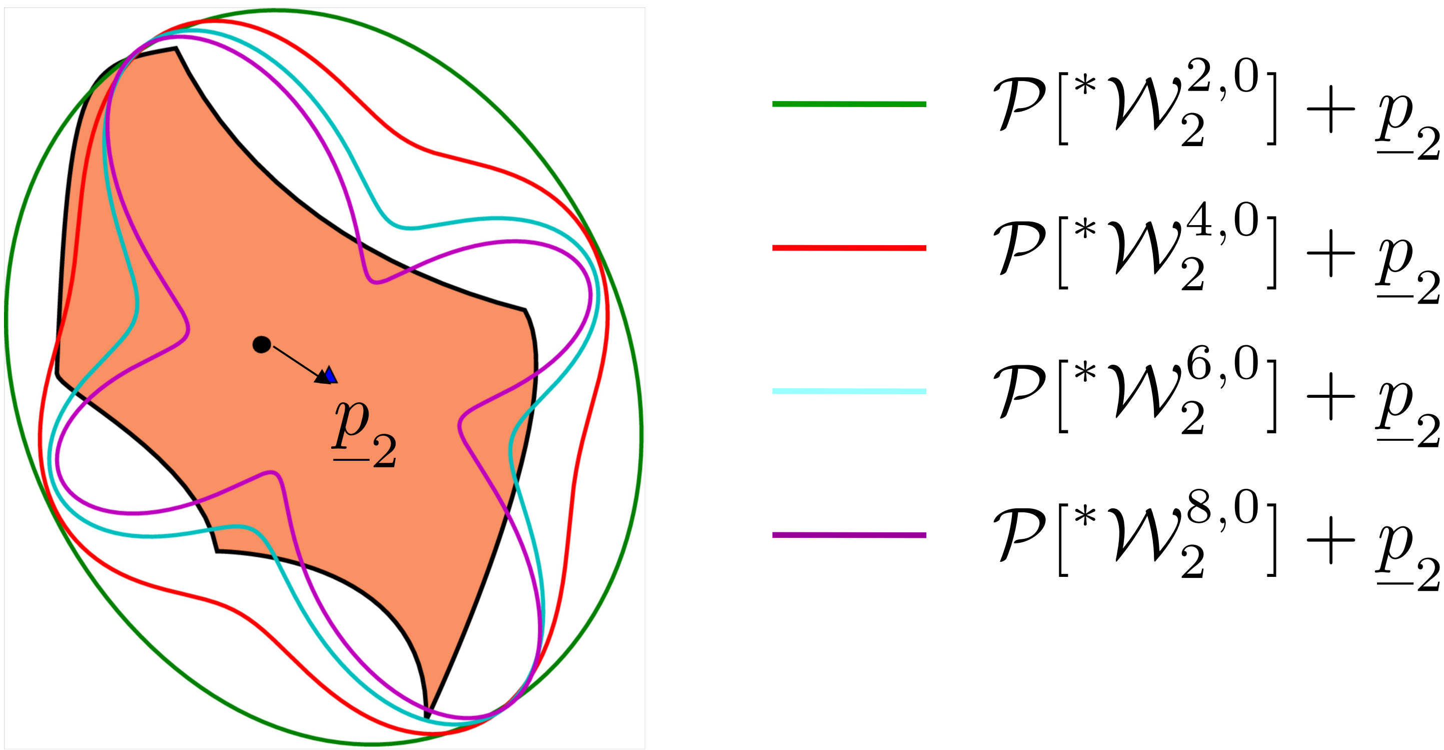
$$\mathcal{W}_2^{r,s} = \int_{\partial\Omega_\alpha} \kappa(\underline{x}) \underline{x}^{\otimes^r} \odot [\underline{n}(\underline{x})]^{\otimes^s} \mathrm{d}S$$



Single grain morphology characterization

For a single grain, there are many different Minkowski tensors of a given order, most of which are independent.

Example: Reynolds glyphs of curvature-weighted tensors $\mathcal{W}_2^{r,0}$:



Question: What types and orders of Minkowski tensors are relevant and sufficient metrics for a grain?

Classic FFT solver

Following Moulinec and Suquet (1998), we have:

$$\widehat{\mathbf{N}}(\underline{k}) = [\underline{k}\,\mathbb{C}_0\,\underline{k}]^{-1} \quad \forall\, \underline{k} \neq \underline{0}$$

$$\widehat{\mathbf{\Gamma}}(\underline{k}) = \underline{k} \odot \widehat{\mathbf{N}}(\underline{k}) \odot \underline{k} \quad \forall\, \underline{k} \neq 0,\ \widehat{\mathbf{\Gamma}}(\underline{0}) = \mathbb{O}$$

$${}^{0}\boldsymbol{\varepsilon}(\underline{y}) = \langle \boldsymbol{\varepsilon} \rangle,\ \ {}^{0}\boldsymbol{\sigma}(\underline{y}) = \mathbb{C}(\underline{y}) : {}^{0}\boldsymbol{\varepsilon}(\underline{y})$$

$$m = 0,\ \ \epsilon = 2\epsilon_{tol}$$

while $\epsilon > \epsilon_{tol}$:

$$\quad {}^{m}\boldsymbol{\tau}(\underline{y}) = {}^{m}\boldsymbol{\sigma}(\underline{y}) - \mathbb{C}_0 : {}^{m}\boldsymbol{\varepsilon}(\underline{y})$$

$$\quad {}^{m}\Delta\widehat{\boldsymbol{\varepsilon}}(\underline{k}) = -\widehat{\mathbf{\Gamma}}(\underline{k}) : \mathcal{F}\{{}^{m}\boldsymbol{\tau}(\underline{y})\}(\underline{k})$$

$$\quad {}^{m+1}\boldsymbol{\varepsilon}(\underline{y}) = \langle \boldsymbol{\varepsilon} \rangle + \mathcal{F}^{-1}\{{}^{m}\Delta\widehat{\boldsymbol{\varepsilon}}(\underline{k})\}(\underline{y})$$

$$\quad {}^{m+1}\boldsymbol{\sigma}(\underline{y}) = \mathbb{C}(\underline{y}) : {}^{m+1}\boldsymbol{\varepsilon}(\underline{y})$$

$$\quad \epsilon = {}^{m+1}\epsilon$$

Version 1

Discrete system:

$$x_1 = \{\, iL_x/N_x \mid i = 0, \ldots, N_x - 1 \}$$

$$x_2 = \{\, iL_y/N_y \mid i = 0, \ldots, N_y - 1 \}$$

$$k_1 = \left\{ \frac{i - N_x/2}{L_x} \,\middle|\, i = 0, \ldots, N_x - 1 \right\}$$

$$k_2 = \left\{ \frac{i}{L_y} \,\middle|\, i = 0, \ldots, N_y/2 \right\}$$

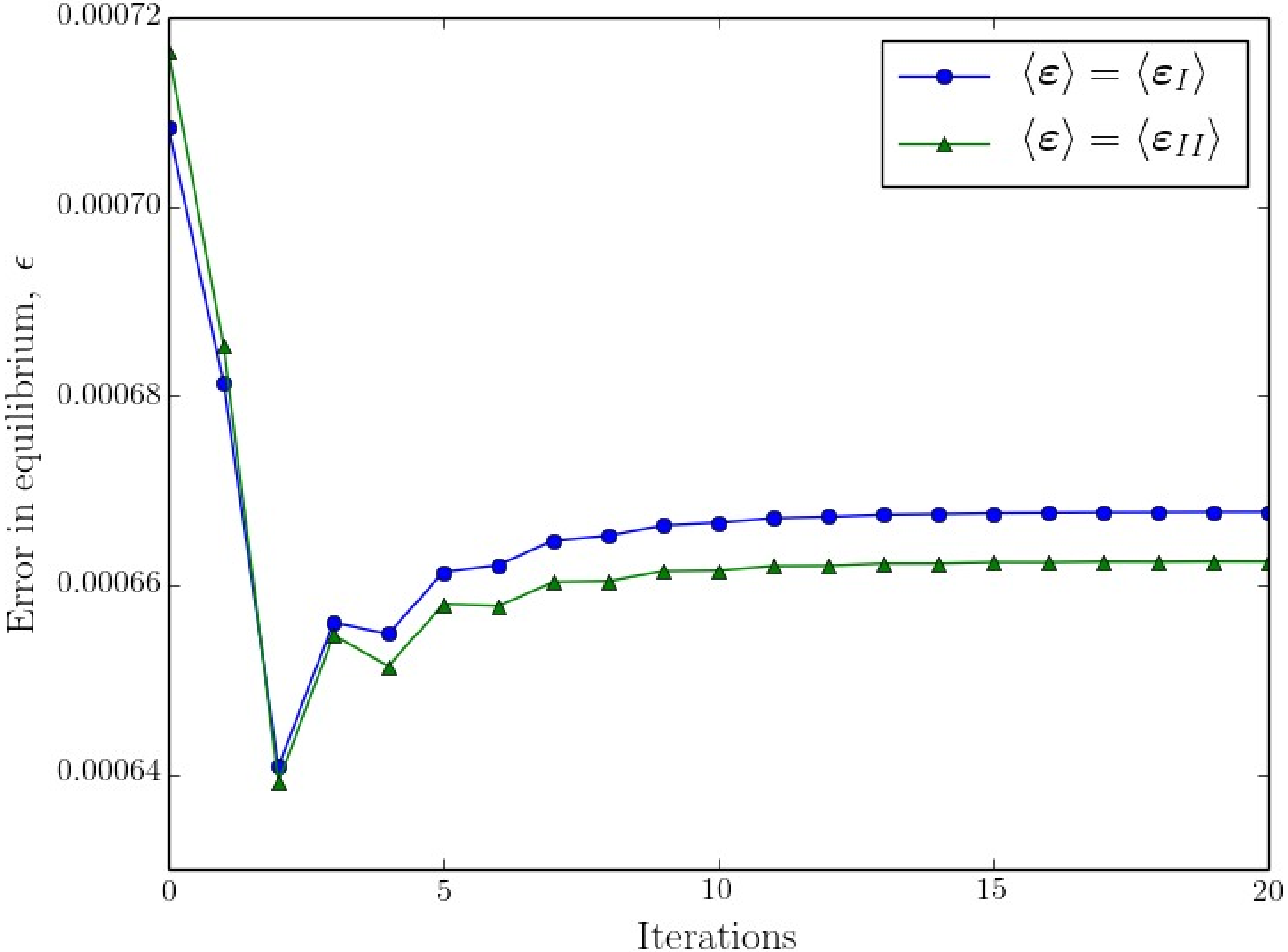
Error in equilibrium:

$${}^{m}\epsilon = \left[\frac{\langle \| {}^{m}\widehat{\boldsymbol{\sigma}}(\underline{k})\,\underline{k} \|^2 \rangle}{{}^{m}\widehat{\boldsymbol{\sigma}}(\underline{0}) : {}^{m}\widehat{\boldsymbol{\sigma}}(\underline{0})} \right]^{1/2}$$

(1) Convergence depends on contrast between phases, and $\mathbb{C}_0$.
(2) Can not solve for infinite contrasts, i.e. rigid/compliant phases.
(3) Numerical homogenization requires several numerical tests.

Convergence – Issues encountered

1) Increasing error vs number of iterations (also observed by Lebensohn, 2001).



$$N_x \times N_y = 2000 \times 2000$$

$$\mathbb{C}_0 = \langle \mathbb{C} \rangle$$

$$\langle \boldsymbol{\varepsilon}_I \rangle = 10^{-5} \underline{e}_1 \otimes \underline{e}_1$$

$$\langle \boldsymbol{\varepsilon}_{II} \rangle = 10^{-5} \underline{e}_2 \otimes \underline{e}_2$$

2) Some cases of instability, e.g. isotropic matrix-fiber w/ much stiffer fiber.

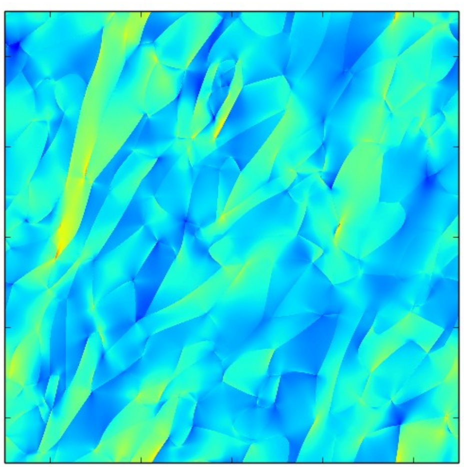
Numerical homogenization (strain-based)

We solve for $\widetilde{\mathbb{C}}$ such that $\langle \boldsymbol{\sigma} \rangle = \widetilde{\mathbb{C}} : \langle \boldsymbol{\varepsilon} \rangle$. From the Hill-Mandel principle, we have:

$$\begin{aligned} \langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle = \widetilde{C}_{1111} \langle \varepsilon_{11} \rangle^2 + \widetilde{C}_{2222} \langle \varepsilon_{22} \rangle^2 + 4\widetilde{C}_{1212} \langle \varepsilon_{12} \rangle^2 \\ + 2\widetilde{C}_{1122} \langle \varepsilon_{11} \rangle \langle \varepsilon_{22} \rangle + 4\widetilde{C}_{1112} \langle \varepsilon_{11} \rangle \langle \varepsilon_{12} \rangle \\ + 4\widetilde{C}_{2212} \langle \varepsilon_{22} \rangle \langle \varepsilon_{12} \rangle \end{aligned}$$

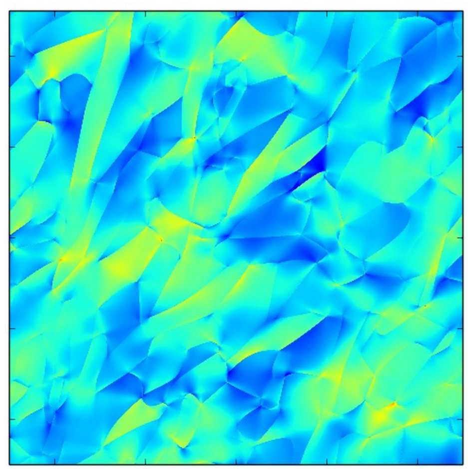
Consider three mean-field loading cases:

$\langle \boldsymbol{\varepsilon}_I \rangle = \langle \varepsilon_{11} \rangle \underline{e}_1 \otimes \underline{e}_1$



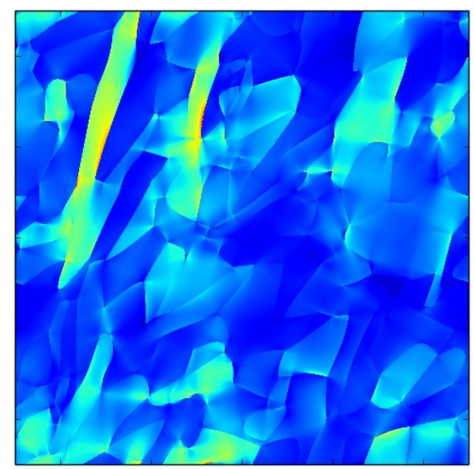
$\boldsymbol{\sigma}_I, \boldsymbol{\varepsilon}_I$

$\langle \boldsymbol{\varepsilon}_{II} \rangle = \langle \varepsilon_{22} \rangle \underline{e}_2 \otimes \underline{e}_2$



$\boldsymbol{\sigma}_{II}, \boldsymbol{\varepsilon}_{II}$

$\langle \boldsymbol{\varepsilon}_{III} \rangle = \langle \varepsilon_{12} \rangle \underline{e}_1 \overset{s}{\otimes} \underline{e}_2$



$\boldsymbol{\sigma}_{III}, \boldsymbol{\varepsilon}_{III}$

Numerical homogenization (strain-based)

Then, from these three loading cases, we have:

$$\widetilde{C}_{1111} = \frac{\langle \boldsymbol{\sigma}_I : \boldsymbol{\varepsilon}_I \rangle}{\langle \varepsilon_{11} \rangle^2} \qquad \widetilde{C}_{2222} = \frac{\langle \boldsymbol{\sigma}_{II} : \boldsymbol{\varepsilon}_{II} \rangle}{\langle \varepsilon_{22} \rangle^2} \qquad \widetilde{C}_{1212} = \frac{\langle \boldsymbol{\sigma}_{III} : \boldsymbol{\varepsilon}_{III} \rangle}{4\langle \varepsilon_{12} \rangle^2}$$

Also, by superposition, we have:

$$\widetilde{C}_{1122} = \frac{\langle (\boldsymbol{\sigma}_I + \boldsymbol{\sigma}_{II}) : (\boldsymbol{\varepsilon}_I + \boldsymbol{\varepsilon}_{II}) \rangle - \widetilde{C}_{1111}\langle \varepsilon_{11} \rangle^2 - \widetilde{C}_{2222}\langle \varepsilon_{22} \rangle^2}{2\langle \varepsilon_{11} \rangle \langle \varepsilon_{22} \rangle}$$

$$\widetilde{C}_{1112} = \frac{\langle (\boldsymbol{\sigma}_I + \boldsymbol{\sigma}_{III}) : (\boldsymbol{\varepsilon}_I + \boldsymbol{\varepsilon}_{III}) \rangle - \widetilde{C}_{1111}\langle \varepsilon_{11} \rangle^2 - 4\widetilde{C}_{1212}\langle \varepsilon_{12} \rangle^2}{4\langle \varepsilon_{11} \rangle \langle \varepsilon_{12} \rangle}$$

$$\widetilde{C}_{2212} = \frac{\langle (\boldsymbol{\sigma}_{II} + \boldsymbol{\sigma}_{III}) : (\boldsymbol{\varepsilon}_{II} + \boldsymbol{\varepsilon}_{III}) \rangle - \widetilde{C}_{2222}\langle \varepsilon_{22} \rangle^2 - 4\widetilde{C}_{1212}\langle \varepsilon_{12} \rangle^2}{4\langle \varepsilon_{22} \rangle \langle \varepsilon_{12} \rangle}$$

Moduli for elastic anisotropy

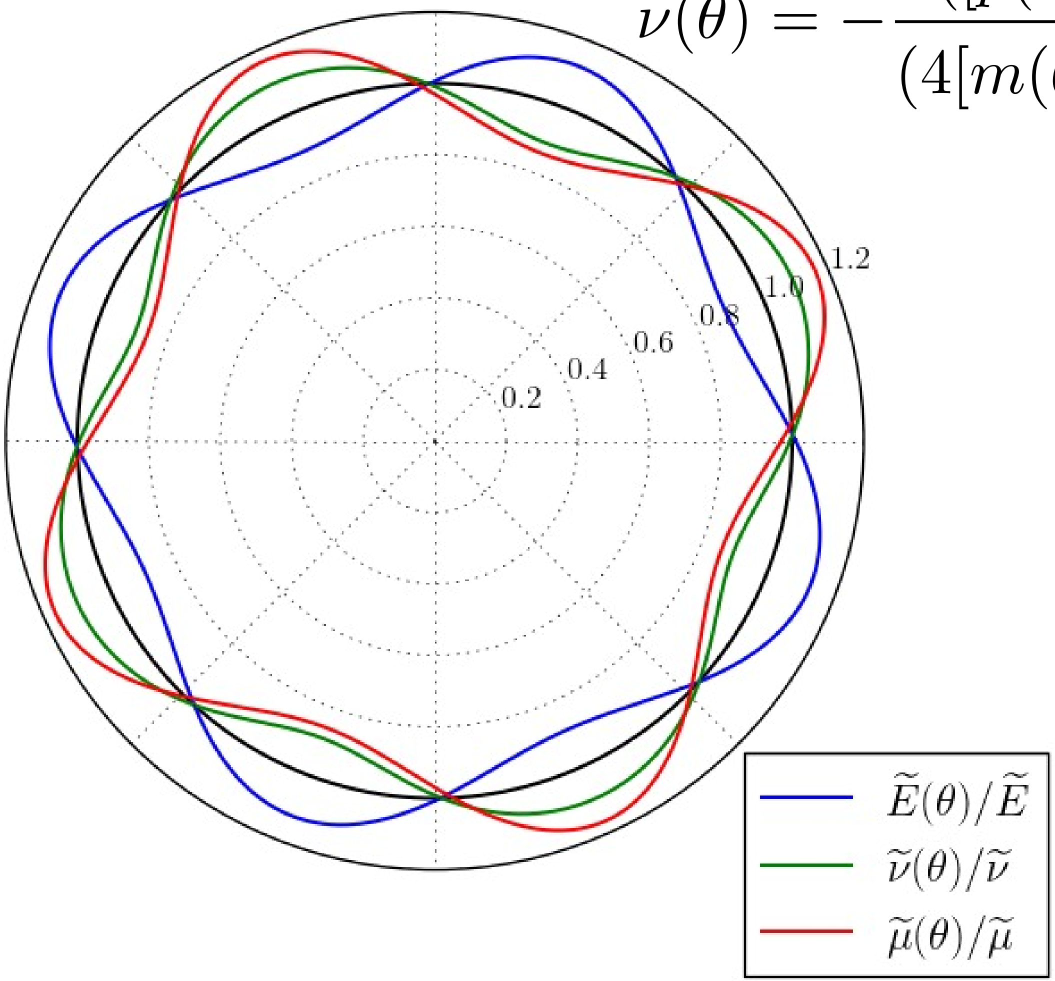
Following Hayes (1972), we have the following moduli:

$$\widetilde{E}(\theta) = ([m(\theta) \otimes m(\theta)] : \widetilde{\mathbb{C}}^{-1} : [m(\theta) \otimes m(\theta)])^{-1}$$

$$\widetilde{\mu}(\theta) = (4[m(\theta) \otimes p(\theta)] : \widetilde{\mathbb{C}}^{-1} : [m(\theta) \otimes p(\theta)])^{-1}$$

and Poisson's ratio:

$$\widetilde{\nu}(\theta) = -\frac{([p(\theta) \otimes p(\theta)] : \widetilde{\mathbb{C}}^{-1} : [m(\theta) \otimes m(\theta)])^{-1}}{(4[m(\theta) \otimes m(\theta)] : \widetilde{\mathbb{C}}^{-1} : [m(\theta) \otimes m(\theta)])^{-1}}$$



$$\widetilde{E} = \frac{1}{2\pi}\int_0^{2\pi} \widetilde{E}(\theta)\mathrm{d}\theta$$

$$\widetilde{\mu} = \frac{1}{2\pi}\int_0^{2\pi} \widetilde{\mu}(\theta)\mathrm{d}\theta$$

$$\widetilde{\nu} = \frac{1}{2\pi}\int_0^{2\pi} \widetilde{\nu}(\theta)\mathrm{d}\theta$$

Mean-field elastic self-consistent homogenization

The following interaction law is assumed between the overall mean strain state $\langle \boldsymbol{\varepsilon} \rangle$ and each local mean field $\langle \boldsymbol{\varepsilon} \rangle_\alpha$:

$$\langle \boldsymbol{\varepsilon} \rangle_\alpha = \widehat{\mathbb{T}}_\alpha : \langle \boldsymbol{\varepsilon} \rangle$$

where $\widehat{\mathbb{T}}_\alpha$ is a strain concentration tensor given by

$$\widehat{\mathbb{T}}_\alpha = [\mathbb{I} + \widehat{\mathbb{P}}^\alpha : (\mathbb{C}_\alpha - \widehat{\mathbb{C}})]^{-1}$$

The Hill-polarization tensor $\widehat{\mathbb{P}}_\alpha$ is computed after the assumption that Ω_α is idealized as an ellipsoid $\widehat{\Omega}_\alpha$:

$$\widehat{\mathbb{P}}^\alpha = \widehat{\mathbb{P}}^\alpha(\underline{x}) = \int_{\widehat{\Omega}_\alpha} \mathcal{F}^{-1} \left\{ \underline{\xi} \odot [\underline{\xi}\, \widehat{\mathbb{C}}\, \underline{\xi}]^{-1} \odot \underline{\xi} \right\} (\underline{x} - \underline{y}) \mathrm{d}V_{\underline{y}}$$

Computed after Masson (2008)

The apparent stiffness is solved for iteratively from:

$$\widehat{\mathbb{C}} = \sum_{\alpha=1}^{n} c_\alpha \mathbb{C}_\alpha : \widehat{\mathbb{T}}_\alpha$$

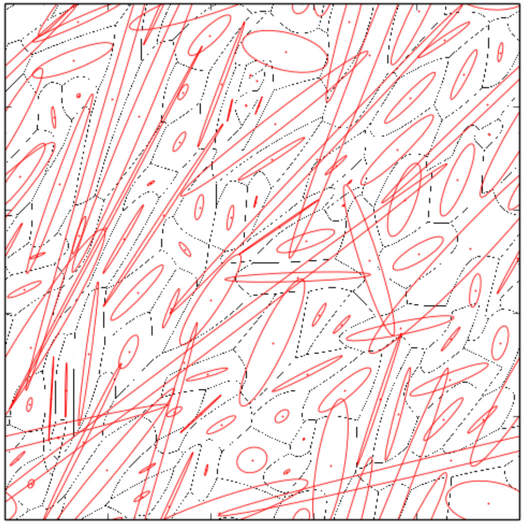
An arbitrary Ω_α can be idealized by many different ellipsoids $\widehat{\Omega}_\alpha$.

What morphological idealization gives best estimates $\widehat{\mathbb{C}}$?

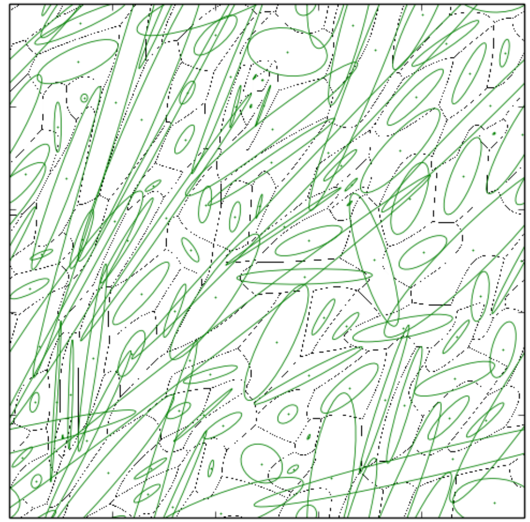
Different morphological idealizations

From each characterization with 2nd order Minkowski tensors:

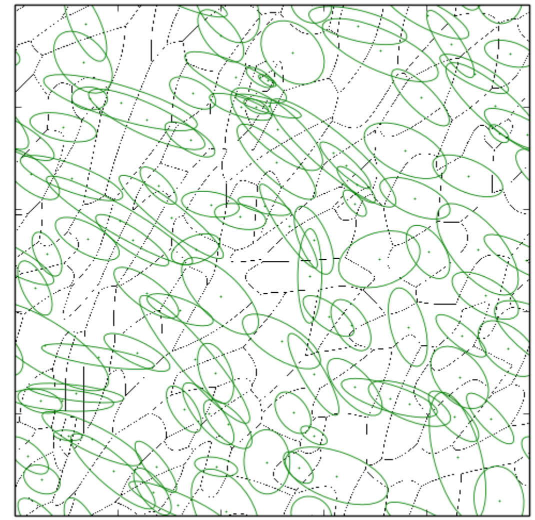
$\mathbf{W}_0^{2,0}$



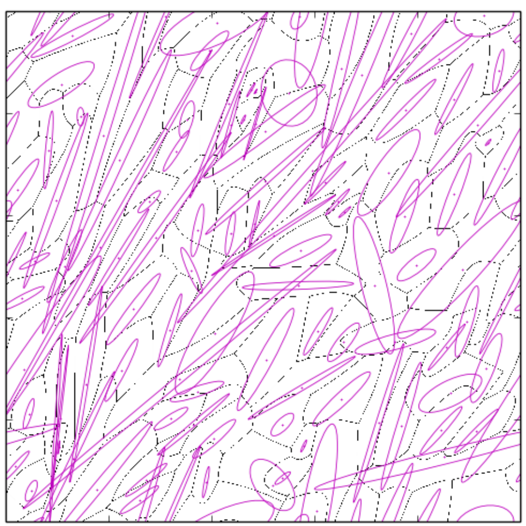
$\mathbf{W}_1^{2,0}$



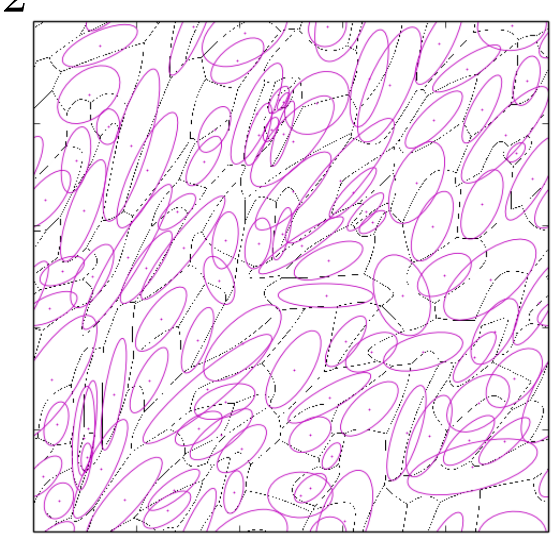
$\mathbf{W}_1^{0,2}$



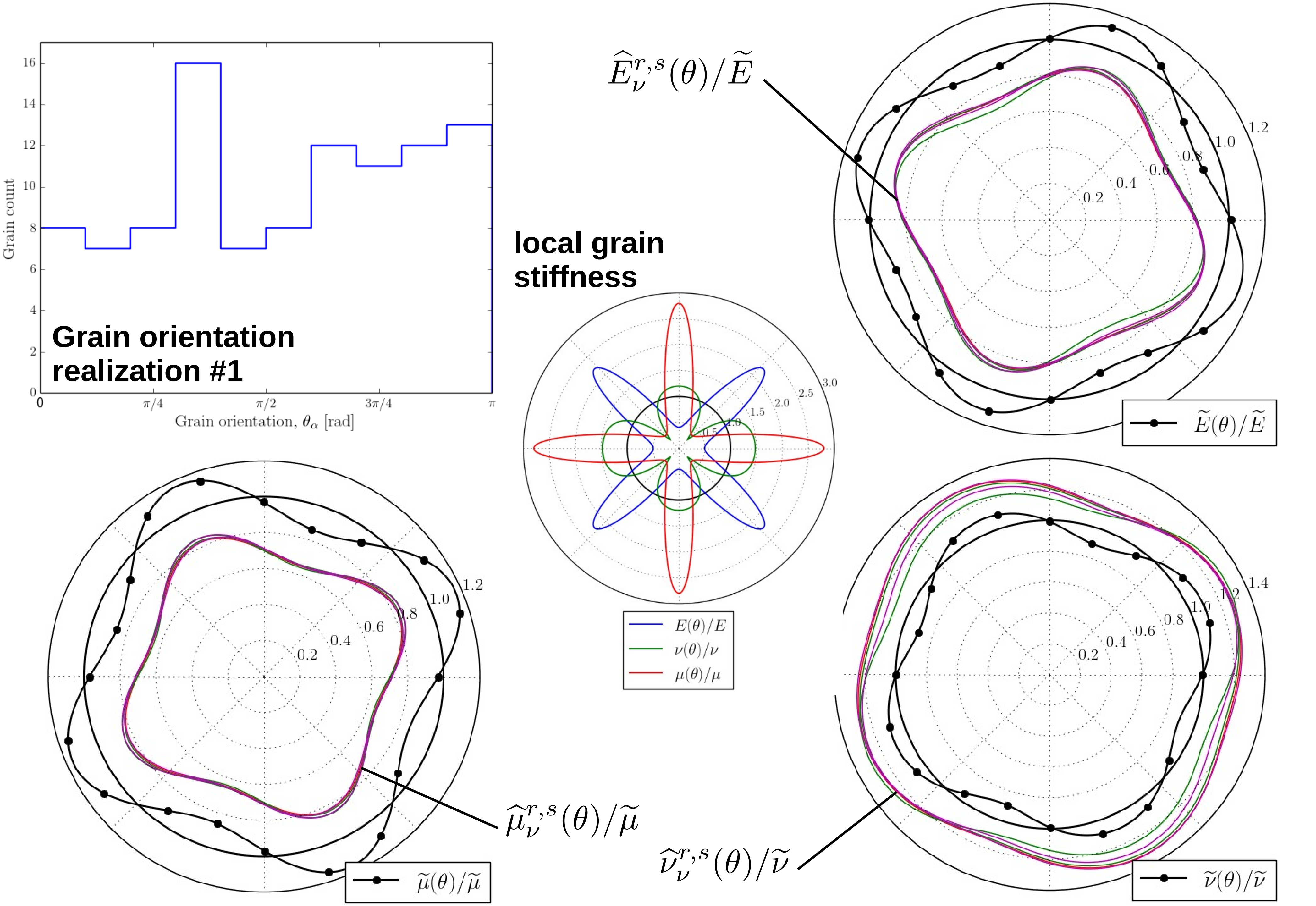
$\mathbf{W}_2^{2,0}$



$\mathbf{W}_2^{1,1}$



Comparison of SC-based elastic stiffness estimates



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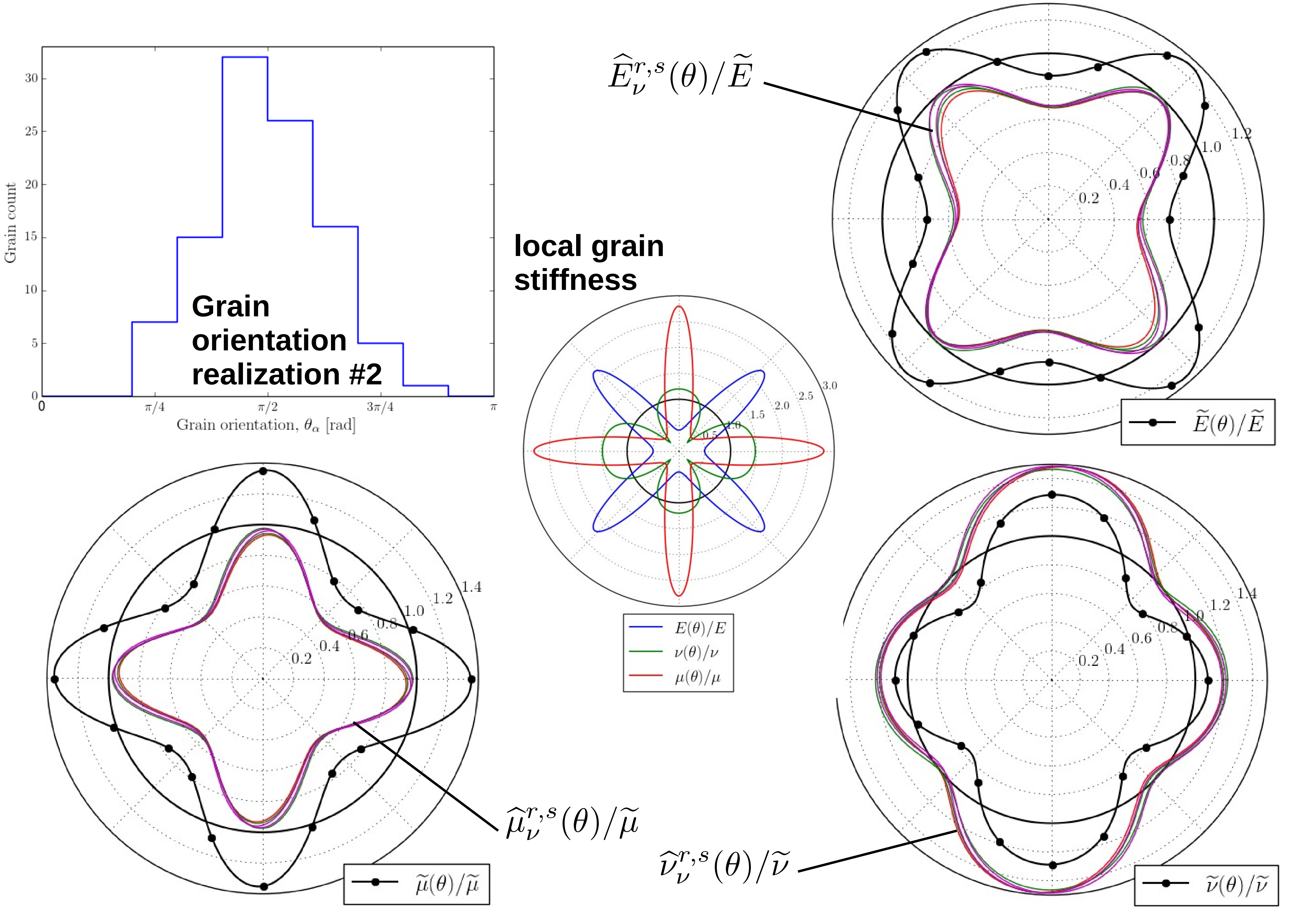

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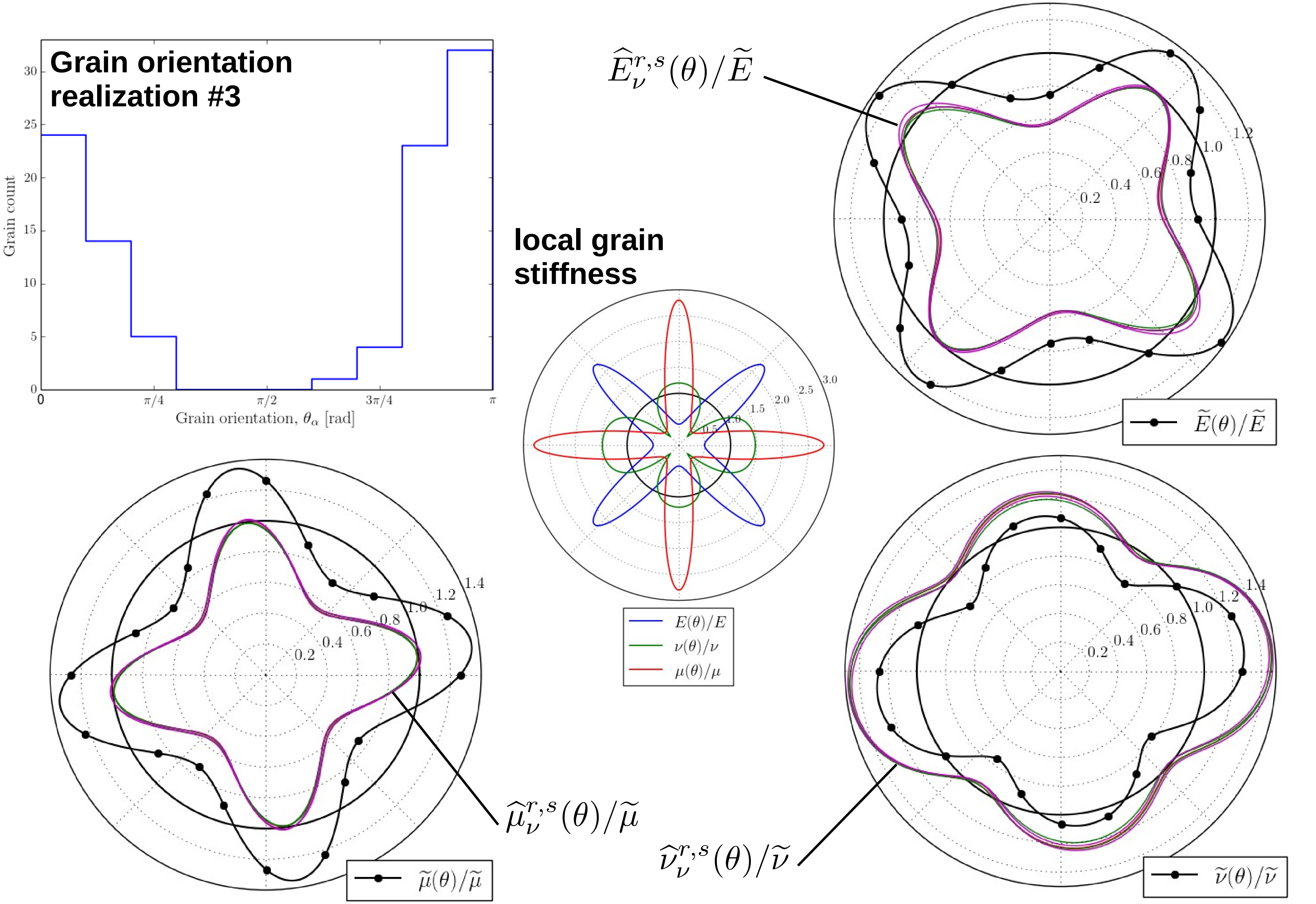

Conclusion

- Morphological characterization of single grains
- Numerical homogenization
- Self-consistent homogenization
- Shape idealization
- Comparison of SC estimates of elastic stiffness

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