Parametric representation, morphological characterization and Eshelby tensor field analysis of planar ellipsoidal growth structures (EGS)

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Presentation outline

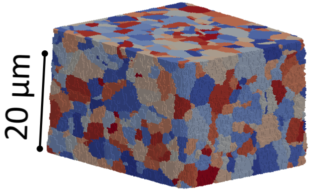
1. Introduction,
2. Definitions of ellipsoidal growth structures (EGS),
3. Parametric representation of planar EGS,
4. Characterization of cell morphology using Minkowski tensors,
5. Eshelby tensor field analysis.

Advantage of a parametric representation

Case of the digitalized data set of a sample of polycrystalline nickel super-alloy IN100 microstructure, see Teferra and Graham-Brady (2015):

Data set from EBSD:

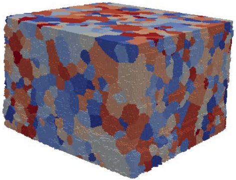
- Data consuming;
- Finite resolution.



4, 444, 713 parameters

Parameterization by ellispoidal growth tessellation

- Less than 2% the original amount of data;
- Infinite resolution (in theory).

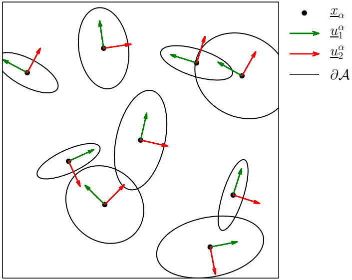


14, 118 parameters

Ellipsoidal growth structures (EGS) — Definitions

An EGS requires:

1. A non-intersecting closed surface $\partial\mathcal{A}$ (or plane curve) with interior $\mathcal{A}$.
2. Two sets $\omega = \{1, ..., N\}$ and $\Omega = \{(\underline{x}_\alpha, \mathbf{Z}_\alpha) \,|\, \alpha \in \omega\}$ such that:
   - every $\underline{x}_\alpha$ is in $\mathcal{A}$,
   - $\underline{x}_\alpha = \underline{x}_\gamma$ if and only if $\alpha = \gamma$,
   - every $\mathbf{Z}_\alpha \in \mathbb{R}^d \times \mathbb{R}^d$ is such that $\underline{x} \cdot \mathbf{Z}_\alpha \cdot \underline{x} > 0$ for all $\underline{x} \neq \underline{0}$.
3. A set of rules after which the EGS is assembled.



We have, $\mathbf{Z}_\alpha = \sum_{j=1}^{d} \frac{\underline{u}_j^\alpha \otimes \underline{u}_j^\alpha}{(v_j^\alpha)^2}$ where v_j^α is a growth velocity along $\underline{u}_j^\alpha$.

Ellipsoidal growth structures (EGS) — Definitions

To define curves and points necessary to construct EGS, we introduce

$$\begin{aligned} \varphi_\alpha &: S^1 \times (0, \Delta) \to S_\alpha \subset \mathbb{R}^2 \\ &: (\underline{x}, t) \mapsto \underline{x}_\alpha + t\,\mathbf{Z}_\alpha^{-1/2} \cdot \underline{x} \end{aligned}$$

where $(0, \Delta)$ is time. Just as φ_α, the inverse

$$\begin{aligned} \varphi_\alpha^{-1} &: S_\alpha \to S^1 \times (0, \Delta) \\ &: \underline{y} \mapsto \left(\frac{\mathbf{Z}_\alpha^{1/2} \cdot (\underline{y} - \underline{x}_\alpha)}{\|\mathbf{Z}_\alpha^{1/2} \cdot (\underline{y} - \underline{x}_\alpha)\|}, \|\mathbf{Z}_\alpha^{1/2} \cdot (\underline{y} - \underline{x}_\alpha)\| \right) \end{aligned}$$

is injective and continuously differentiable so that $S_\alpha = \varphi_\alpha(S^1 \times (0, \Delta))$ is a diffeomorphic transformation of $S^1 \times (0, \Delta)$.

A diffeomorphism φ_α exists for every pair $(\underline{x}_\alpha, \mathbf{Z}_\alpha)$ in Ω.

For Δ large enough, $S_\alpha \cap S_\gamma$ is non-empty. For every such set, we define $\mathcal{I}_{\alpha\gamma} \subset S_\alpha \cap S_\gamma$ as follows:

$$\mathcal{I}_{\alpha\gamma} = \{\underline{y} \in S_\alpha \cap S_\gamma \mid f_\gamma^\alpha(\underline{y}) = 0\}$$

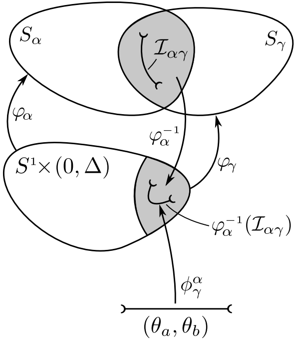
Ellipsoidal growth structures (EGS) — Definitions

$\mathcal{I}_{\alpha\gamma}$ are common curves and constitute the essential geometrical components of planar EGS.

$f_\gamma^\alpha : S_\alpha \cap S_\gamma \to \mathbb{R}$ is defined after the type of structure wanted for an implicit representation of $\mathcal{I}_{\alpha\gamma}$.

For an explicit representation, we study $\varphi_\alpha^{-1}(\mathcal{I}_{\alpha\gamma})$ instead of $\mathcal{I}_{\alpha\gamma}$.

We obtain a representation of the form $\varphi_\alpha \circ \phi_\gamma^\alpha : (\theta_a, \theta_b) \to \mathcal{I}_{\alpha\gamma}$ after 1D parameterizations $\phi_\gamma^\alpha : (\theta_a, \theta_b) \to \varphi_\alpha^{-1}(\mathcal{I}_{\alpha\gamma})$ are constructed.



Case of tessellation – Local parameterizations

For tessellations, the common curves $\mathcal{I}_{\alpha\gamma}$ are implicitly defined using

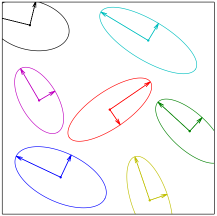
$$f_\gamma^\alpha(\underline{y}) = \tau \circ \varphi_\alpha^{-1}(\underline{y}) - \tau \circ \varphi_\gamma^{-1}(\underline{y})$$

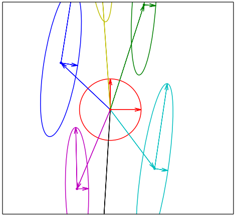
where τ is a projection on time.

The corresponding spatial projection is

$$\pi \circ \varphi_\alpha^{-1}(\mathcal{I}_{\alpha\gamma}) = \{\underline{x} \in S^1 \mid [\underline{x} - \underline{x}_\gamma^\alpha(t)]^{\otimes^2} : \mathbf{Z}_\gamma^\alpha = 1,\ t \in (0, \Delta)\}$$

where $\underline{x}_\gamma^\alpha(t) \equiv \pi \circ \varphi_\alpha^{-1}(\underline{x}_\gamma) = t^{-1}\mathbf{Z}_\alpha^{1/2} \cdot (\underline{x}_\gamma - \underline{x}_\alpha)$ and $\mathbf{Z}_\gamma^\alpha = \mathbf{Z}_\alpha^{-1/2} \cdot \mathbf{Z}_\gamma \cdot \mathbf{Z}_\alpha^{-1/2}$ so that $\pi \circ \varphi_\alpha^{-1}(\mathcal{I}_{\alpha\gamma})$ is the set of all the points in S^1 intersected by an ellipse of fixed shape moving towards the center of the unit circle during the time $(0, \Delta)$:





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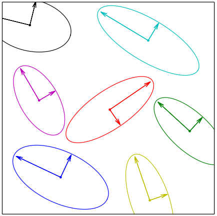

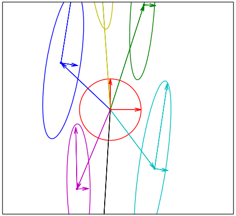

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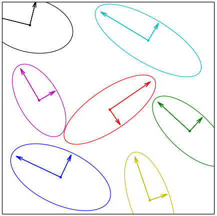

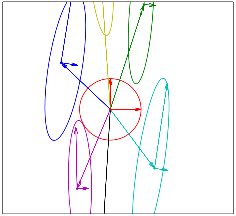

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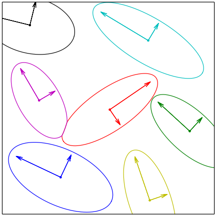

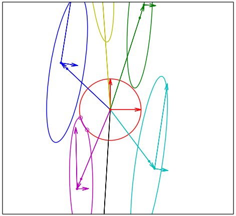

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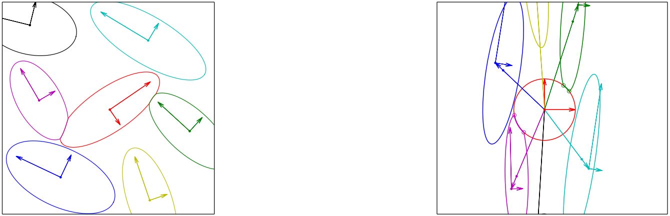

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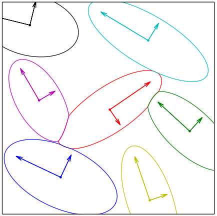

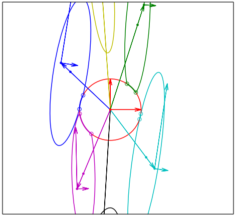

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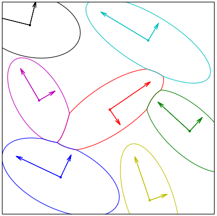

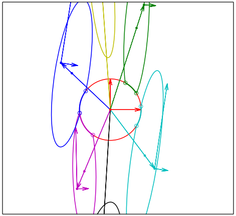

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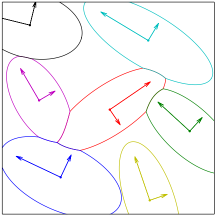

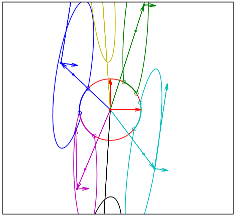

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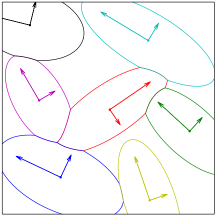

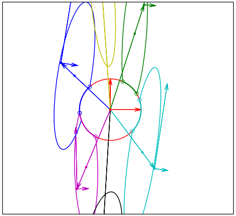

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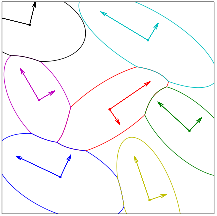

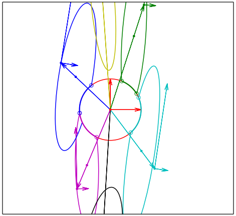

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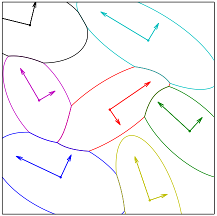

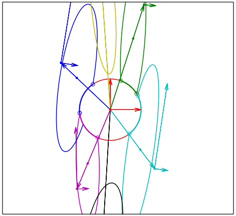

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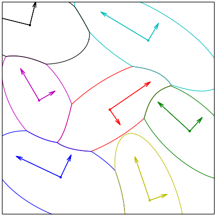
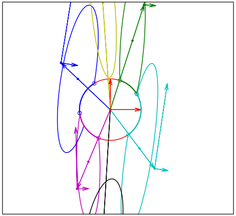




Case of tessellation – Local parameterizations

The local charts

$$\phi_\gamma^\alpha : (\theta_a, \theta_b) \to V \subset S^1 \times (0, \Delta)$$
$$: \theta \mapsto (\underline{x}(\theta), \xi_\gamma^\alpha \circ \underline{x}(\theta))$$

are obtained by geometric construction where $\underline{x}(\theta)$ is a curve on S^1 and ξ_γ^α is a *contact function* given by

$$\xi_\gamma^\alpha \circ \underline{x}(\theta) = \frac{\underline{x}_\gamma^\alpha \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha}{\underline{x}(\theta) \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha + \delta\sqrt{\left(\underline{x}(\theta) \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha\right)^2 - \left(\underline{x}_\gamma^\alpha \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha\right)\left[\underline{x}(\theta) \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}(\theta) - 1\right]}}.$$

The specification of $\underline{x}(\theta)$, δ and the ranges of these parameterizations depend on the pairwise interaction between α and γ characterized by

$$c_\gamma^\alpha = \|\underline{x}_\gamma^\alpha\|^{-1}\sqrt{(v_2^{\alpha\gamma}\underline{u}_1^{\alpha\gamma} \cdot \underline{x}_\gamma^\alpha)^2 + (v_1^{\alpha\gamma}\underline{u}_2^{\alpha\gamma} \cdot \underline{x}_\gamma^\alpha)^2}$$

Every parameterization is changed to $\hat{\phi}_\gamma^\alpha : \theta \mapsto (\hat{\underline{x}}(\theta - \rho_\gamma^\alpha), \xi_\gamma^\alpha \circ \hat{\underline{x}}(\theta - \rho_\gamma^\alpha))$ where $\hat{\underline{x}}(\theta) = \underline{u}_1^\alpha \cos\theta + \underline{u}_2^\alpha \sin\theta$ and

$$U = \begin{cases} [-\pi, \theta_b + \rho_\gamma^\alpha) \cup (\theta_a + \rho_\gamma^\alpha + 2\pi, \pi) & \text{if } \theta_a + \rho_\gamma^\alpha < -\pi, \\ [-\pi, \theta_b + \rho_\gamma^\alpha - 2\pi) \cup (\theta_a + \rho_\gamma^\alpha, \pi) & \text{if } \theta_b + \rho_\gamma^\alpha \geq \pi, \\ (\theta_a + \rho_\gamma^\alpha, \theta_b + \rho_\gamma^\alpha) & \text{otherwise}, \end{cases}$$

with $\rho_\gamma^\alpha = \mathrm{sgn}(\underline{u}_2^\alpha \cdot \underline{x}(0))\mathrm{acos}(\underline{u}_1^\alpha \cdot \underline{x}(0))$.

Definition of the tessellation from cell boundaries

For every $\alpha \in \omega$, we define a tessellation cell $\mathcal{C}_\alpha$ as the interior of a closed curve $\partial\mathcal{C}_\alpha$ such that $\cup_{\alpha\in\omega}\mathcal{C}_\alpha = \mathcal{A}$ and $\mathcal{C}_\alpha \cap \mathcal{C}_\gamma = \emptyset$ for every $\alpha \neq \gamma$. Every tessellation cell is simply connected.

1) Radially convex cells ("easy case"): Define prior contact curves as follows:

$$\partial\mathcal{C}_{\alpha i} = \left\{ \varphi_\alpha(\underline{x}, \xi^\alpha_{\omega^\alpha(i)}(\underline{x})) \mid \underline{x} \in S^1 \text{ and } \xi^\alpha_{\omega^\alpha(i)}(\underline{x}) = \min_{\gamma\in\omega\setminus\alpha} \xi^\alpha_\gamma(\underline{x}) \right\}$$

where $\omega^\alpha : \{1, \ldots, n^\alpha_c\} \rightarrow \omega$ maps a contact i of the cell α to a corresponding neighboring cell γ.

The number of prior contacts n^α_c is the cardinality of $\cap_{i=1}^{n^\alpha_c} \pi \circ \varphi_\alpha^{-1}(\partial\mathcal{C}_{\alpha i})$.

Every prior contact curve $\partial\mathcal{C}_{\alpha i}$ is a subset of a corresponding common curve $\tilde{\mathcal{I}}_{\alpha\omega^\alpha(i)}$.

One neighboring cell can be responsible for more than one contact.

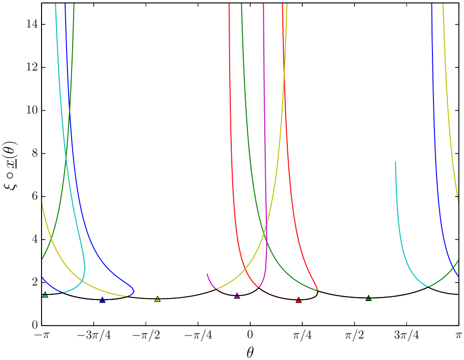
Definition of the tessellation from cell boundaries

Radially convexity occurs when the set

$$\mathcal{K}_\alpha = \{(\underline{x}, t) \in S^1 \times (0, \Delta) \mid (\underline{x}, t) = \varphi_\alpha^{-1}(\partial\mathcal{C}_{\alpha i}) \cap \varphi_\alpha^{-1}(\partial\mathcal{C}_{\alpha j}),\ i \neq j\}$$

has cardinality n_c^α. Then, a tessellation cell $\mathcal{C}_\alpha$ can be defined as the interior of the Jordan curve with trace

$$\partial\mathcal{C}_\alpha = \bigcup_{i=1}^{n_c^\alpha} \partial\mathcal{C}_{\alpha i}.$$



Definition of the tessellation from cell boundaries

2) Non-radially convex cells ("difficult case"):

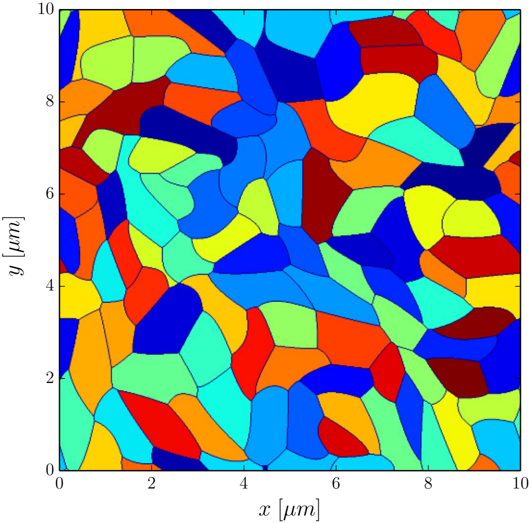
$\mathcal{K}_\alpha$ has cardinality lower than n_c^α, $\partial\mathcal{C}_\alpha$ is not a closed curve.

This means there is at least one pair (i,j) such that
$\pi \circ \varphi_\alpha^{-1}(\partial\mathcal{C}_{\alpha i}) \cap \pi \circ \varphi_\alpha^{-1}(\partial\mathcal{C}_{\alpha j}) \neq \emptyset$ while
$\tau \circ \varphi_\alpha^{-1}(\partial\mathcal{C}_{\alpha i}) \cap \tau \circ \varphi_\alpha^{-1}(\partial\mathcal{C}_{\alpha j}) = \emptyset$.

We say that the cell is *not* radially convex at $\underline{x}_\alpha$.

Examples of space-filling planar EGS – Tessellation 1

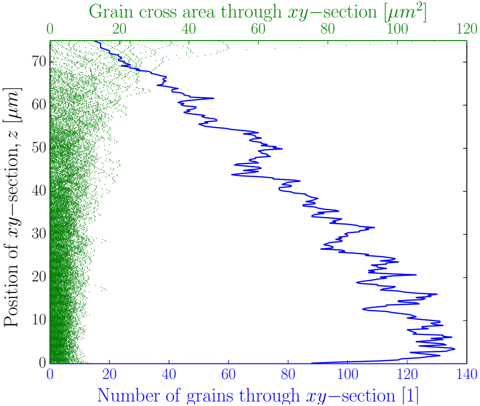
Marked point process simulated after a packing algorithm with explicitly prescribed correlations.

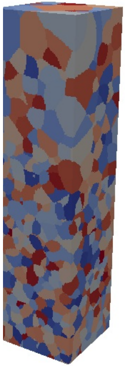


Examples of space-filling spatial EGS – Tessellation 2

Example of a functionally-graded microstructure realization obtained after appropriate selection of parameter distributions and correlations.

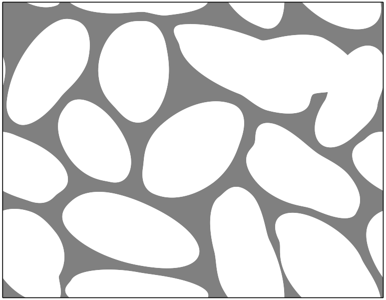
Marked point process simulated after Teferra and Graham-Brady (2015)



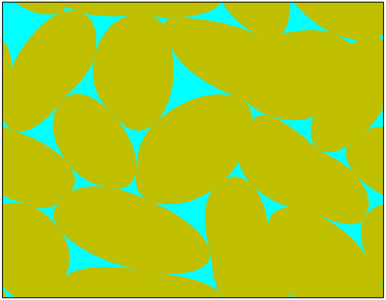


Other examples of planar EGS

Foam structure:



Granular media:



The cells $\mathcal{C}_\alpha$ are cellular pores and solid grains, respectively. For each case, the corresponding contact functions are bounded by $0 < \xi \leq \tilde{\xi}$ where $\tilde{\xi}$ is the corresponding contact function obtained for tessellations.

Local characterization of a cell boundary

At every non-singular point $\underline{y}$ of a cell boundary $\partial\mathcal{C}_\alpha$, we have a unit tangent given by

$$\underline{t}(\theta) = \frac{\partial_\theta \varphi_\alpha \circ \phi_\gamma^\alpha(\theta)}{\|\partial_\theta \varphi_\alpha \circ \phi_\gamma^\alpha(\theta)\|} = \frac{A(\theta)\underline{u}_1^\alpha + B(\theta)\underline{u}_2^\alpha}{\sqrt{A(\theta)^2 + B(\theta)^2}}$$

where A and B depend on the locally defined contact function:

$$A(\theta) = v_1^\alpha \left[\dot{\xi}(\theta)\cos\theta - \xi(\theta)\sin\theta\right] \quad \text{and} \quad B(\theta) = v_2^\alpha \left[\dot{\xi}(\theta)\sin\theta + \xi(\theta)\cos\theta\right].$$

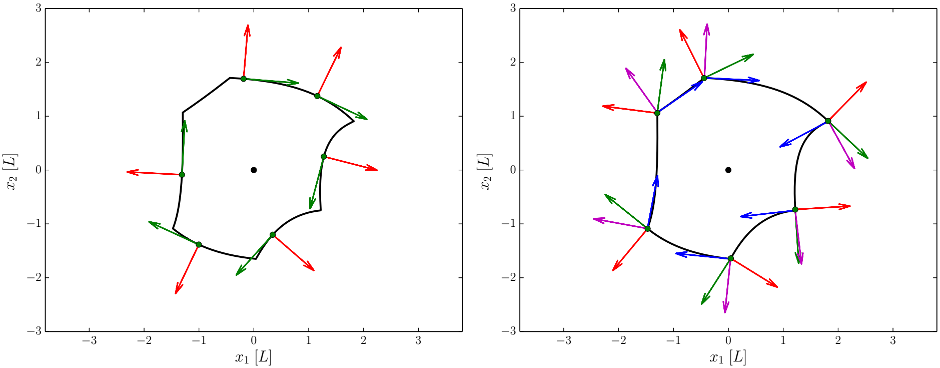
The corresponding unit normal is

$$\underline{n}(\theta) = \mathbf{R}_{\pi/2}^t \cdot \underline{t}(\theta) = \frac{B(\theta)\underline{u}_1^\alpha - A(\theta)\underline{u}_2^\alpha}{\sqrt{A(\theta)^2 + B(\theta)^2}}$$

and the signed curvature is

$$\kappa(\theta) = \frac{\xi^2(\theta) - \xi(\theta)\ddot{\xi}(\theta) + 2\dot{\xi}^2(\theta)}{\left[\dot{\xi}^2(\theta) + \xi^2(\theta)\right]^{3/2}}.$$

Local characterization of a cell boundary



Minkowski tensors of the 0th kind

Minkowski tensors of the 0th kind measure how area is distributed inside $\mathcal{C}_\alpha$:

$$\mathcal{W}_0^{r,0}(\mathcal{C}_\alpha) \equiv \int_{\mathcal{C}_\alpha} \underline{x}^{\otimes^r} \, \mathrm{d}A$$

Using our parameterization of $\partial\mathcal{C}_\alpha$, we obtain

$$\mathcal{W}_0^{r,0}(\mathcal{C}_\alpha) = \sum_{i=0}^{r} \sum_{j=0}^{r-i} \binom{r}{i+j} \underline{x}_\alpha^{\otimes^{r-i-j}} \odot \underline{u}_1^{\alpha\otimes^i} \odot \underline{u}_2^{\alpha\otimes^j} I_0^{i,j}(\mathcal{C}_\alpha)$$

where the scalar integral $I_0^{i,j}$ is given by

$$I_0^{i,j}(\mathcal{C}_\alpha) \equiv \binom{i+j}{i} \frac{(v_1^\alpha)^{i+1}(v_2^\alpha)^{j+1}}{i+j+2} \sum_{n=1}^{n_\alpha} \int_{\theta_a}^{\theta_b} [\xi(\theta)]^{i+j+2} (\cos\theta)^i (\sin\theta)^j \mathrm{d}\theta.$$

where the terms within the integral are defined locally for every chart.

Minkowski tensors of the 1st kind

Minkowski tensors of the 1st kind measure how boundary points and their orientation are distributed in $\partial\mathcal{C}_\alpha$:

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

Using our parameterization of $\partial\mathcal{C}_\alpha$, we obtain

$$\mathcal{W}_1^{r,s}(\mathcal{C}_\alpha) = \sum_{i=0}^{r} \sum_{j=0}^{r-i} \sum_{k=0}^{s} \binom{r}{i+j} \binom{s}{k} \underline{x}_\alpha^{\otimes^{r-i-j}} \odot \underline{u}_1^{\alpha^{\otimes^{s+i-k}}} \odot \underline{u}_2^{\alpha^{\otimes^{j+k}}} I_1^{i,j,k,s-k}(\mathcal{C}_\alpha)$$

where the scalar integral $I_1^{i,j,k,\ell}$ is given by

$$I_1^{i,j,k,\ell}(\mathcal{C}_\alpha) \equiv (-1)^k \binom{i+j}{j} (v_1^\alpha)^i (v_2^\alpha)^j \sum_{n=1}^{n_\alpha} \int_{\theta_a}^{\theta_b} \frac{[\xi(\theta)]^{i+j} (\cos\theta)^i (\sin\theta)^j \, [A(\theta)]^k \, [B(\theta)]^\ell}{\left\{[A(\theta)]^2 + [B(\theta)]^2\right\}^{\frac{k+\ell-1}{2}}} \mathrm{d}\theta.$$

where the terms within the integral are defined locally for every chart.

Minkowski tensors of the 2nd kind

Minkowski tensors of the 2nd kind measure how curvature is distributed along boundary points and their orientation in $\partial\mathcal{C}_\alpha$:

$$\mathcal{W}_2^{r,s} \equiv \int_{\partial\mathcal{C}_\alpha} \kappa(\underline{x})\underline{x}^{\otimes^r} \odot [\underline{n}(\underline{x})]^{\otimes^s} \mathrm{d}\ell + \sum_{\underline{y}\in\mathcal{K}_\alpha} \mathcal{D}^{r,s}(\underline{y})$$

where $\mathcal{D}^{r,s}$ are contributions due to curvature jumps at common points.

Using our parameterization of $\partial\mathcal{C}_\alpha$, we obtain

$$\mathcal{W}_2^{r,s}(\mathcal{C}_\alpha) = \sum_{i=0}^{r}\sum_{j=0}^{r-i}\sum_{k=0}^{s} \binom{r}{i+j}\binom{s}{k} \underline{x}_\alpha^{\otimes^{r-i-j}} \odot \underline{u}_1^{\alpha\,\otimes^{s+i-k}} \odot \underline{u}_2^{\alpha\,\otimes^{j+k}} I_2^{i,j,k,s-k}(\mathcal{C}_\alpha) + \sum_{\underline{y}\in\mathcal{K}_\alpha} \mathcal{D}^{r,s}(\underline{y})$$

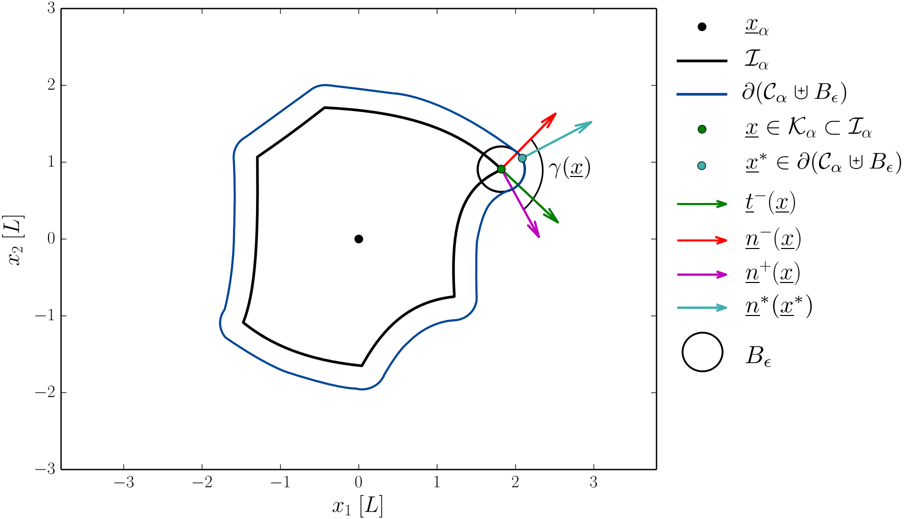
where the scalar integral $I_2^{i,j,k,\ell}$ is given by

$$I_2^{i,j,k,\ell}(\mathcal{C}_\alpha) \equiv (-1)^k \binom{i+j}{j} (v_1^\alpha)^i (v_2^\alpha)^j \sum_{n=1}^{n_\alpha} \int_{\theta_a}^{\theta_b} \frac{[\xi(\theta)]^{i+j} (\cos\theta)^i (\sin\theta)^j \, [A(\theta)]^k \, [B(\theta)]^\ell}{\{[A(\theta)]^2 + [B(\theta)]^2\}^{\frac{k+\ell-1}{2}}} \, \kappa(\theta)\, \mathrm{d}\theta$$

where, once again, the terms within the integral are defined locally for every chart.

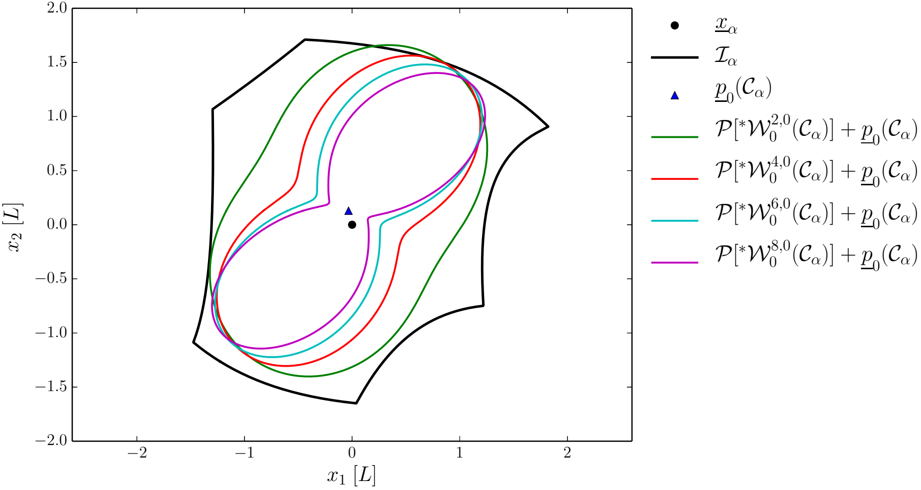
Minkowski tensors of the 2nd kind

Discontinuity terms $\mathcal{D}^{r,s}$ are obtained using a parallel body construction



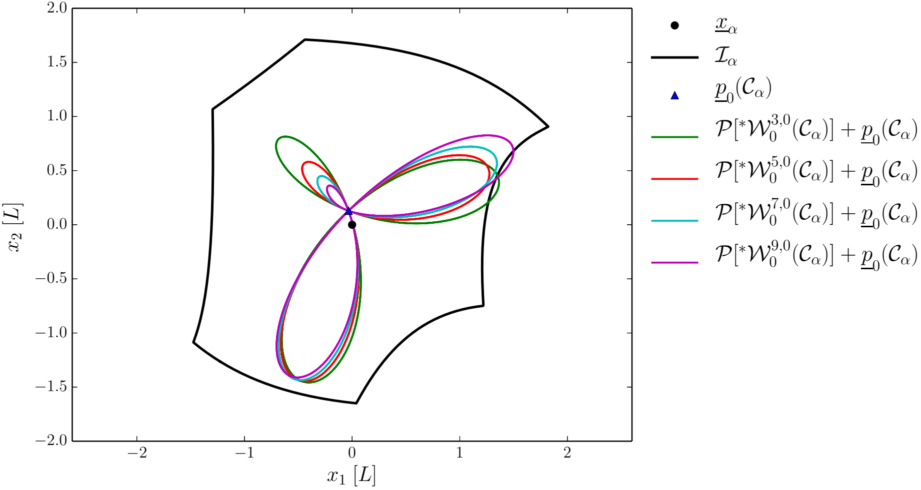
Morphological characterization of a planar cell – (Results)

Radial projections of even $\mathcal{W}_0^{r,0}$:



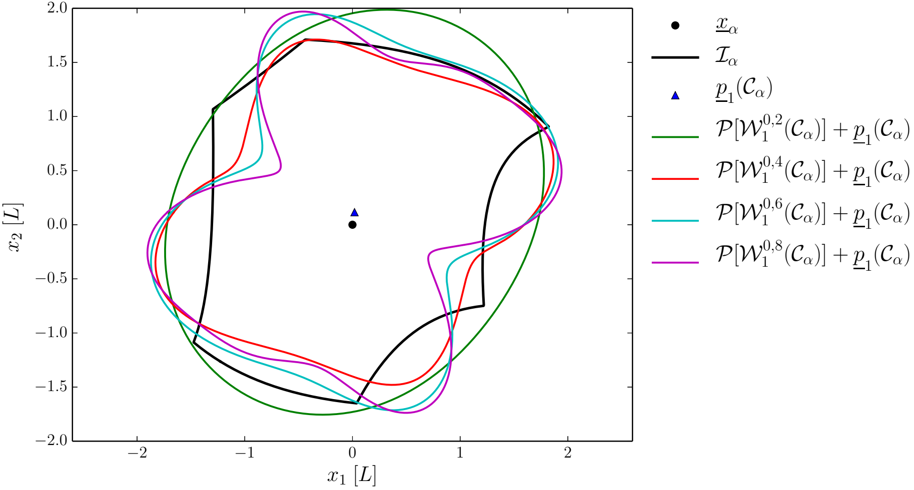
Morphological characterization of a planar cell – Results

Radial projections of odd $\mathcal{W}_0^{r,0}$:



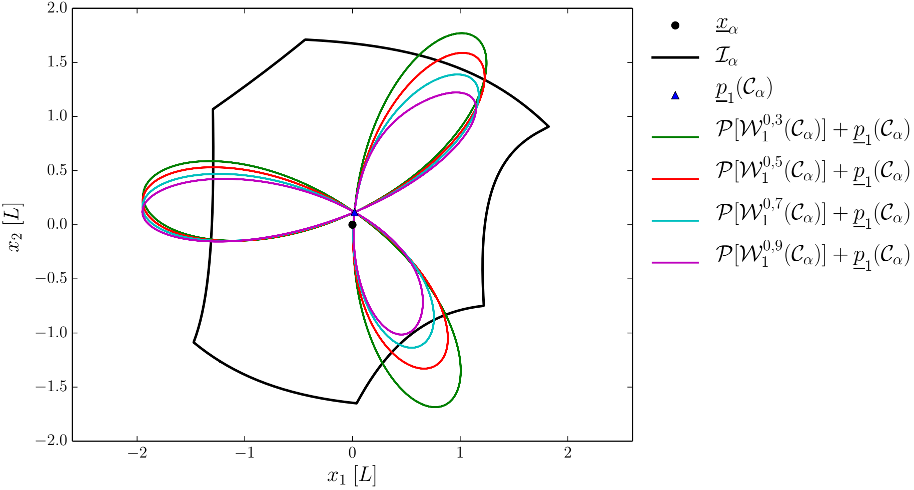
Morphological characterization of a planar cell – Results

Radial projections of even $\mathcal{W}_1^{0,s}$:



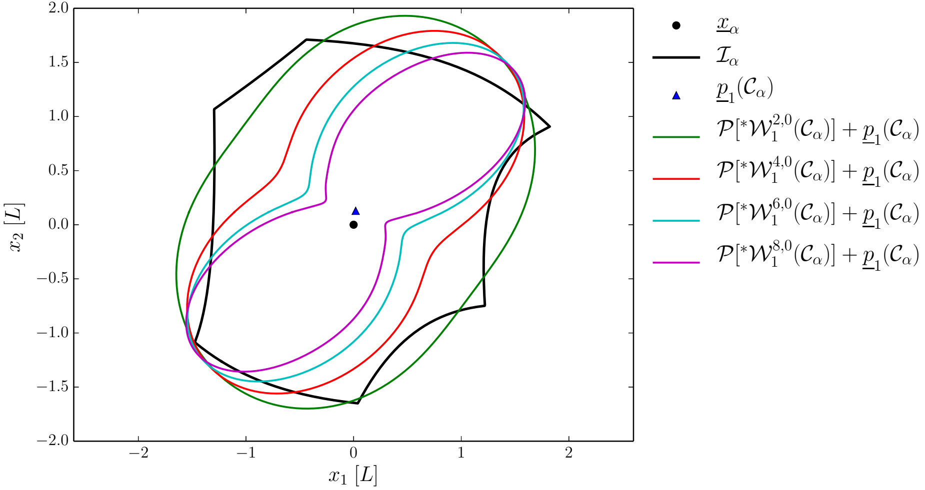
Morphological characterization of a planar cell – Results

Radial projections of odd $\mathcal{W}_1^{0,s}$:



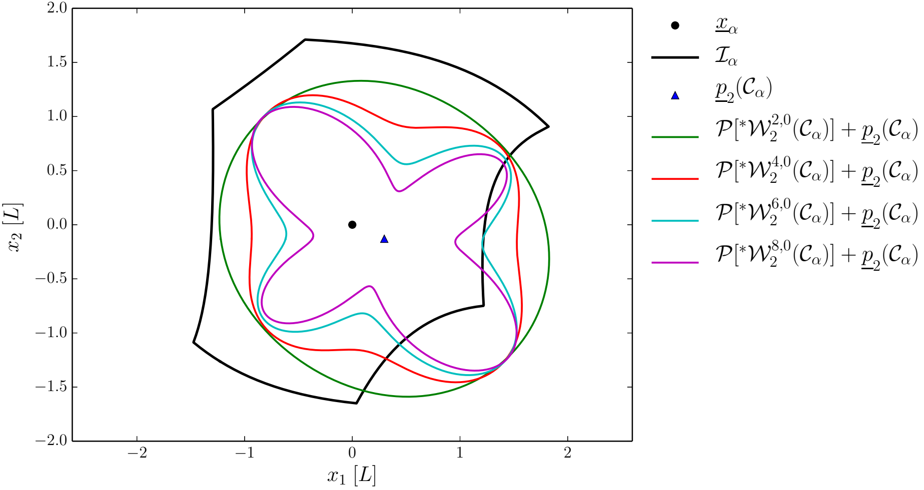
Morphological characterization of a planar cell – Results

Radial projections of even $\mathcal{W}_1^{r,0}$:



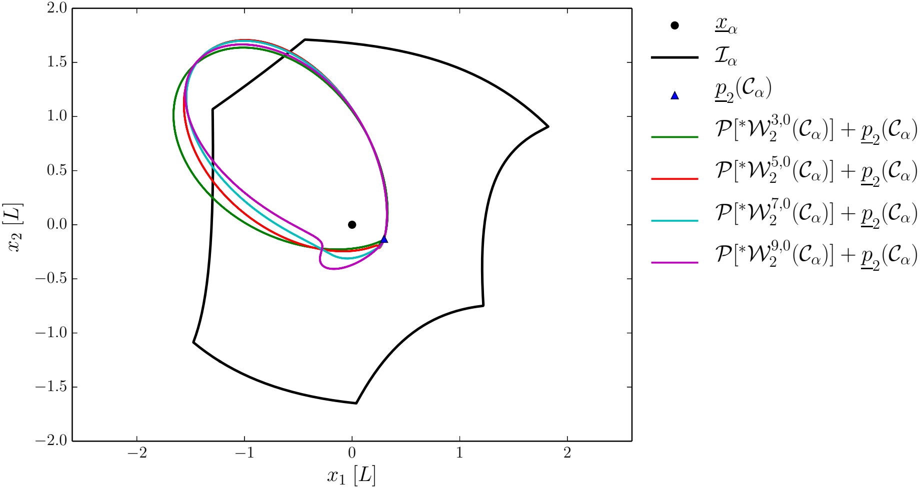
Morphological characterization of a planar cell – Results

Radial projections of even $\mathcal{W}_2^{r,0}$:



Morphological characterization of a planar cell – Results

Radial projections of odd $\mathcal{W}_2^{r,0}$:



Towards a better interpration of Minkowski tensors – $\mathcal{W}_1^{0,s}$

The p.d.f. f of a unit normal $\underline{m}$ in $\partial\mathcal{C}_\alpha$ can be expressed as

$$f(\underline{m}) = \int\limits_{\partial\mathcal{C}^\alpha} \delta(\underline{m} - \underline{n}(\underline{x}))\mathrm{d}\ell$$

which can not be analytically resolved even from our parameterization of $\partial\mathcal{C}_\alpha$. Similarly, the Minkowski tensors $\mathcal{W}_1^{0,s}$ can be considered as moments of this distribution

$$\mathcal{W}_1^{0,s} = \int\limits_{\partial\mathcal{C}^\alpha} [\underline{n}(\underline{x})]^{\otimes^s} f(\underline{n}(\underline{x}))\mathrm{d}\ell.$$

Following Katani (1984), possible ansatz for models of such random normal distributions are

$$F(\underline{m}) = C + \underline{C}\cdot\underline{m} + \mathbf{C} : (\underline{m}\otimes\underline{m}) + \underline{m}\cdot\mathcal{C} : (\underline{m}\otimes\underline{m}) + \ldots$$
$$F(\underline{m}) = [C + \underline{C}\cdot\underline{m} + \mathbf{C} : (\underline{m}\otimes\underline{m}) + \underline{m}\cdot\mathcal{C} : (\underline{m}\otimes\underline{m}) + \ldots]^2$$
$$F(\underline{m}) = \exp[C + \underline{C}\cdot\underline{m} + \mathbf{C} : (\underline{m}\otimes\underline{m}) + \underline{m}\cdot\mathcal{C} : (\underline{m}\otimes\underline{m}) + \ldots]$$

where C, $\underline{C}$, $\mathcal{C}$, ... are yet to be defined.

Towards a better interpration of Minkowski tensors – $\mathcal{W}_1^{0,s}$

Still following Katani (1984), for a given ansatz and error norm to minimize between $f(\underline{n})$ and $F(\underline{x})$, one can derive expressions for C, $\underline{C}$, $\mathcal{C}$, ... in terms of $\mathcal{W}_1^{0,s}$'s.

For example, minimizing the least square error for the first symmetric ($F(-\underline{n}) = F(\underline{n})$) ansatz up to order 4 leads up to

$$F(\underline{n}) = \frac{1}{2\pi}[1 + 4(\mathbf{W}_1^{0,2} - \mathbf{1}/2) : (\underline{n} \otimes \underline{n})] + 16(\underline{n} \otimes \underline{n}) : [\mathbb{W}_1^{0,4} - \mathbf{1} \odot \mathbf{W}_1^{0,2} + \mathbf{1} \odot \mathbf{1}/8] : (\underline{n} \otimes \underline{n})$$

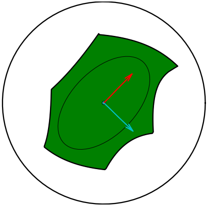
where we recall that $\mathbf{W}_1^{0,2} = \mathbf{1} : \mathbb{W}_1^{0,4}$.

Remarks:

- Considering tensors of odd orders could yield non-symmetric distribution,
- Such methods can be applied to the whole EGS with $\mathcal{W}_1^{0,s}(\cap_\alpha \partial \mathcal{C}_\alpha)$, ...
- Similar random models are used in plastic flow rules and hardening of granular media as well as elastic stiffness prediction of generic porous media – see works of Cowin, Mehrabadi, Nemat-Nasser, ...
- Can we apply similar procedures to other Minkowski tensors?

Eshelby problem and disturbance fields

Let's isolate a grain $\mathcal{C}_\alpha$ from a tessellation and see how it reacts to a uniform eigenstrain ε^0 when embedded in a uniform neighborhood:



Assuming an elastic medium under small def., the eigenstrain maps linearly to a disturbance field:

$$\varepsilon(\underline{y}) = \mathbb{S}(\underline{y}) : \varepsilon^0.$$

For $R \to \infty$, this is the Eshelby problem and $\mathbb{S}(\underline{y})$ is the Eshelby tensor field. For highly symmetric grains in infinite neighborhood, the Eshelby tensor field is uniform inside the inclusion.

Solutions to this problem are a fundamental result as they are commonly invoked to develop both, linear and nonlinear homogenization schemes of heterogeneous media.

Computation of Eshelby tensor fields

In the general case of a finite neighborhoods, $\mathbb{S}(\underline{y})$ is decomposed in

$$\mathbb{S}(\underline{y}) = \mathbb{S}^{\infty}(\underline{y}) + \mathbb{S}^{b}(\underline{y})$$

where $\mathbb{S}^b$ vanishes as $R \to \infty$.
The "inifite contribution" can be expressed as:

$$\mathbb{S}^{\infty}(\underline{y}) = \mathbb{S}^0 \chi^{\alpha}(\underline{y}) + \frac{\kappa - 1}{\kappa + 1} \mathbf{1} \otimes \mathbf{d}^{\infty}(\underline{y}) + 2 \frac{\mathbf{d}^{\infty}(\underline{y}) \otimes \mathbf{1}}{\kappa + 1} + 4 \frac{\mathbb{D}^{\infty}(\underline{y})}{\kappa + 1}$$

where χ^{α} is the indicator function of the cell and $\mathbb{S}^0$ is the isotropic part of $\mathbb{S}^{\infty}$ given by:

$$\mathbb{S}^0 = \underline{u}_1^{\alpha^{\otimes^4}} + \underline{u}_2^{\alpha^{\otimes^4}} + \frac{\kappa - 1}{2(\kappa + 1)} (\underline{u}_1^{\alpha} \odot \underline{u}_2^{\alpha})^{\otimes^2} - \frac{\kappa - 1}{2(\kappa + 1)} \mathbf{1} \otimes \mathbf{1} - \frac{\Re\{(\underline{u}_1^{\alpha} + i \underline{u}_2^{\alpha})^{\otimes^4}\}}{2(\kappa + 1)}$$

κ is the Kolosov's constant.

Computation of Eshelby tensor fields – Infinite contribution

$\mathbf{d}^\infty$ and $\mathbb{D}^\infty$ are given by

$$\mathbf{d}^\bullet \circ \underline{y}(r,\vartheta) = \Re\{\gamma_2^{\alpha,\bullet}(r,\vartheta)\}\Re\{(\underline{u}_1^\alpha + i\underline{u}_2^\alpha)^{\otimes^2}\} + \Im\{\gamma_2^{\alpha,\bullet}(r,\vartheta)\}\Im\{(\underline{u}_1^\alpha + i\underline{u}_2^\alpha)^{\otimes^2}\}$$

$$\mathbb{D}^\bullet \circ \underline{y}(r,\vartheta) = \Re\{\gamma_4^{\alpha,\bullet}(r,\vartheta)\}\Re\{(\underline{u}_1^\alpha + i\underline{u}_2^\alpha)^{\otimes^4}\} + \Im\{\gamma_4^{\alpha,\bullet}(r,\vartheta)\}\Im\{(\underline{u}_1^\alpha + i\underline{u}_2^\alpha)^{\otimes^4}\}$$

where $\underline{y}(r,\vartheta) = r\underline{x}(\vartheta)$ with $\underline{x}(\theta) = \underline{u}_1^\alpha \cos\theta + \underline{u}_2^\alpha \sin\theta$.

Using our parametrization of $\partial\mathcal{C}_\alpha$ and following Zou et al. (2010), the complex potentials $\gamma_2^{\alpha,\infty}$ and $\gamma_4^{\alpha,\infty}$ can be recast in

$$\gamma_2^{\alpha,\infty}(r,\vartheta) = \frac{1}{4\pi i}\int_{\partial\mathcal{C}^\alpha} \frac{[\dot{\xi}(\theta)\underline{x}(\theta) + \xi(\theta)\dot{\underline{x}}(\theta)] \cdot \mathbf{Z}_\alpha^{-1/2} \cdot (\underline{u}_1^\alpha + i\underline{u}_2^\alpha)}{[\underline{x}_\alpha + \xi(\theta)\mathbf{Z}_\alpha^{-1/2} \cdot \underline{x}(\theta) - r\underline{x}(\vartheta)] \cdot (\underline{u}_1^\alpha - i\underline{u}_2^\alpha)} \mathrm{d}\theta$$

and

$$\gamma_4^{\alpha,\infty}(r,\vartheta) = \frac{1}{16\pi i}\int_{\partial\mathcal{C}^\alpha} \frac{\left\{[\underline{x}_\alpha + \xi(\theta)\mathbf{Z}_\alpha^{-1/2} \cdot \underline{x}(\theta) - r\underline{x}(\vartheta)] \otimes [\dot{\xi}(\theta)\underline{x}(\theta) + \xi(\theta)\dot{\underline{x}}(\theta)] \cdot \mathbf{Z}_\alpha^{-1/2}\right\} : (\underline{u}_1^\alpha + i\underline{u}_2^\alpha)^{\otimes^2}}{\{[\underline{x}_\alpha + \xi(\theta)\mathbf{Z}_\alpha^{-1/2} \cdot \underline{x}(\theta) - r\underline{x}(\vartheta)] \cdot (\underline{u}_1^\alpha - i\underline{u}_2^\alpha)\}^2} \mathrm{d}\theta$$

Computation of Eshelby tensor fields – Bounded contribution

Following Zou et al. (2012), we use the following expression for $\mathbb{S}^b(\underline{y})$:

$$\begin{aligned}\mathbb{S}^b(\underline{y}) = \Re\{c_0^{\alpha,b}(\underline{y})\}\frac{\kappa-1}{\kappa+1}\mathbf{1}\otimes\mathbf{1} + \frac{2\Re\{c_1^{\alpha,b}(\underline{y})\}}{\kappa+1}\Re\{(\underline{u}_1^\alpha + i\underline{u}_2^\alpha)^{\otimes^4}\} + \frac{4\Re\{c_1^{\alpha,b}(\underline{y})\}}{\kappa+1}(\underline{u}_1^\alpha\odot\underline{u}_2^\alpha)^{\otimes^2} + \frac{\kappa-1}{\kappa+1}\mathbf{1}\otimes\mathbf{d}^{b_1}(\underline{y}) \\ + \frac{2}{\kappa+1}\mathbf{d}^{b_2}(\underline{y})\otimes\mathbf{1} + \frac{2\Im\{c_1^{\alpha,b}(\underline{y})\}}{\kappa+1}\Im\{(\underline{u}_1^\alpha + i\underline{u}_2^\alpha)^{\otimes^4}\} - \frac{4\Im\{c_1^{\alpha,b}(\underline{y})\}}{\kappa+1}\underline{u}_1^\alpha\odot\underline{u}_2^\alpha\otimes(\underline{u}_1^\alpha\otimes\underline{u}_1^\alpha - \underline{u}_2^\alpha\otimes\underline{u}_2^\alpha)\end{aligned}$$

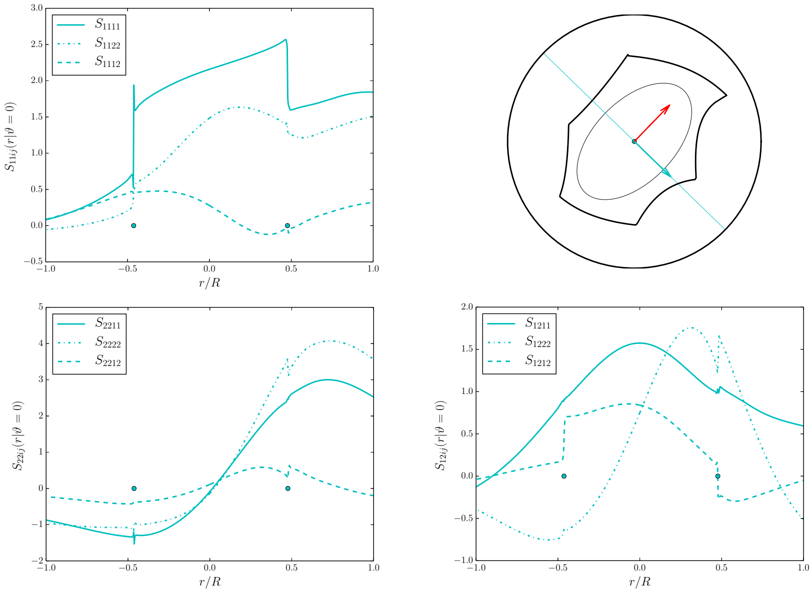
where $c_0^{\alpha,b}$, $c_1^{\alpha,b}$, $\mathbf{d}^{b_1}$ and $\mathbf{d}^{b_2}$ can also be recast in terms of complex integrals specific to our parameterization of $\partial\mathcal{C}_\alpha$.

We isolate analytically the respective real and imaginary part of each of these expressions and perform integrals numerically for a grain.

Remark: To compute the integrals corresponding to the bounded contribution, the type of boundary condition (traction or displacement-free) must be specified. Here, we consider traction free.

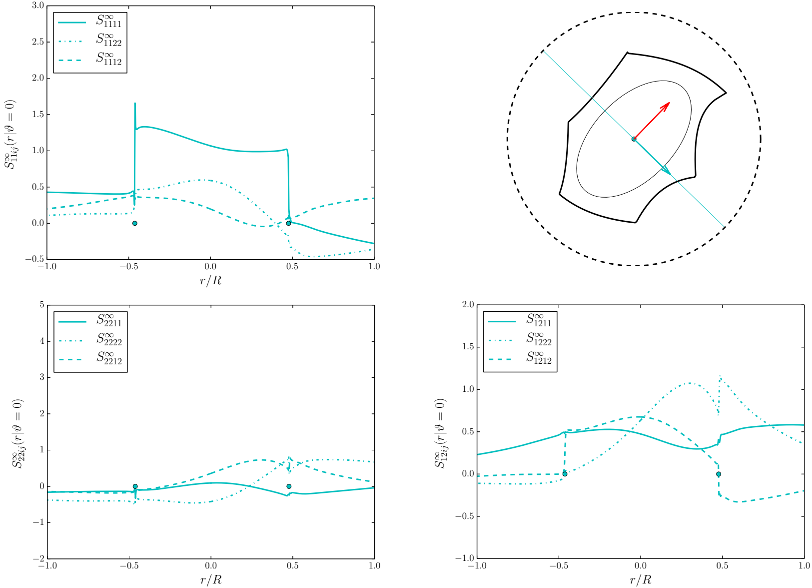
Computation of Eshelby tensor fields – Results for $\mathbb{S}(r|\vartheta)$

Projections along $\underline{u}_1^\alpha$ with basis $\{\underline{u}_1^\alpha, \underline{u}_2^\alpha\}$:



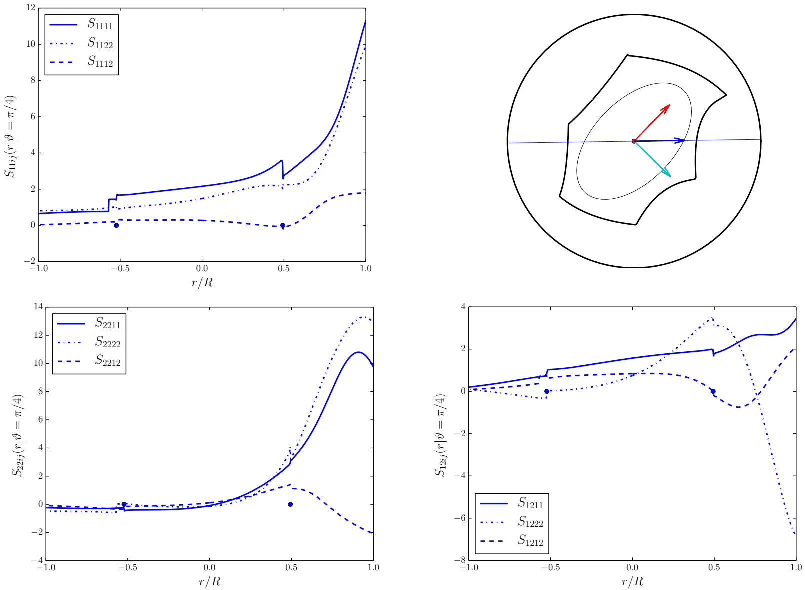
Computation of Eshelby tensor fields – Results for $\mathbb{S}^{\infty}(r|\vartheta)$

Projections along $\underline{u}_1^{\alpha}$ with basis $\{\underline{u}_1^{\alpha}, \underline{u}_2^{\alpha}\}$:



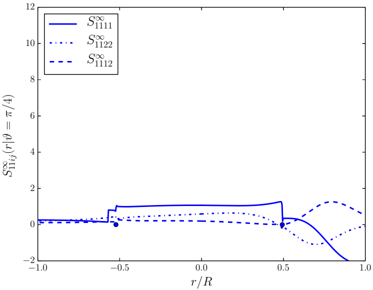
Computation of Eshelby tensor fields – Results for $\mathbb{S}(r|\vartheta)$

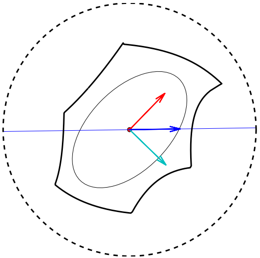
Projections along $\sqrt{2}/2(\underline{u}_1^\alpha + \underline{u}_2^\alpha)$ with basis $\{\underline{u}_1^\alpha, \underline{u}_2^\alpha\}$:

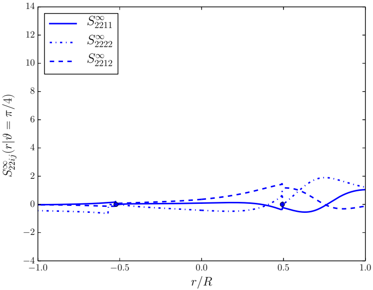


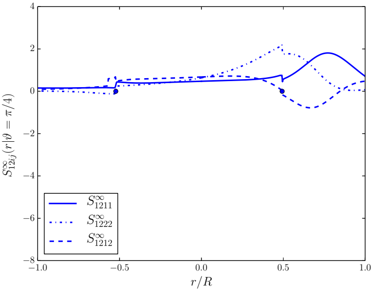
Computation of Eshelby tensor fields – Results for $\mathbb{S}^{\infty}(r|\vartheta)$

Projections along $\sqrt{2}/2(\underline{u}_1^{\alpha} + \underline{u}_2^{\alpha})$ with basis $\{\underline{u}_1^{\alpha}, \underline{u}_2^{\alpha}\}$:



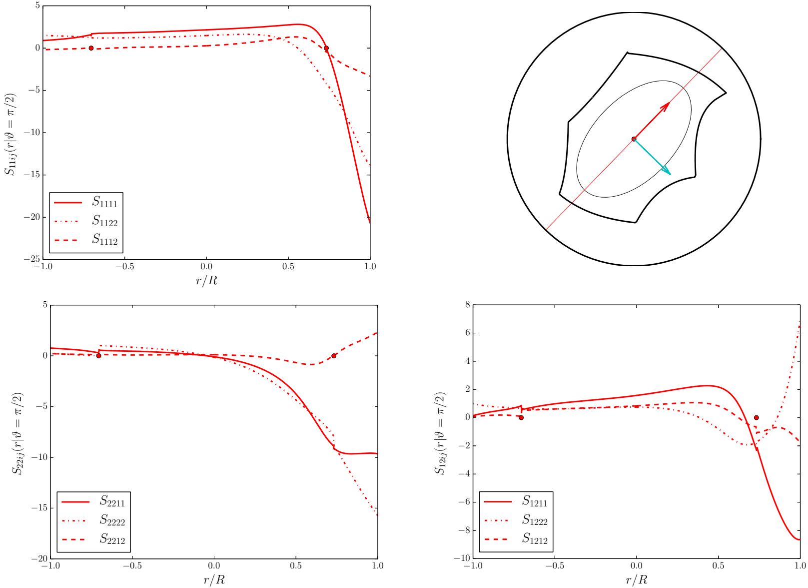






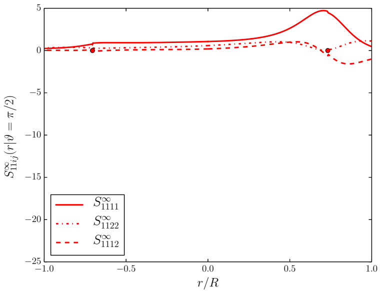
Computation of Eshelby tensor fields – Results for $\mathbb{S}(r|\vartheta)$

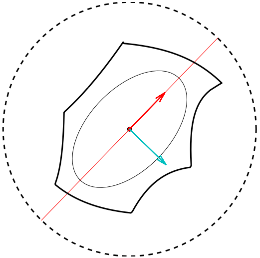
Projections along $\underline{u}_2^\alpha$ with basis $\{\underline{u}_1^\alpha, \underline{u}_2^\alpha\}$:

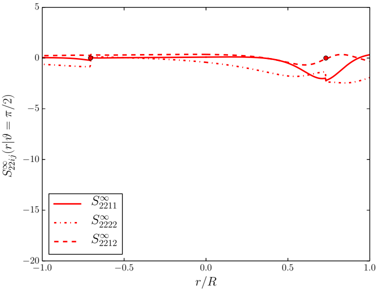


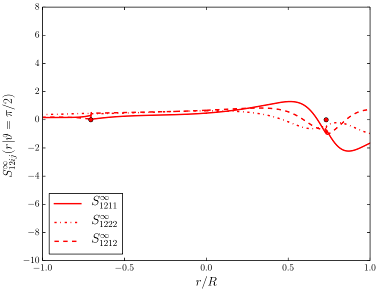
Computation of Eshelby tensor fields – Results for $\mathbb{S}^\infty(r|\vartheta)$

Projections along $\underline{u}_2^\alpha$ with basis $\{\underline{u}_1^\alpha, \underline{u}_2^\alpha\}$:



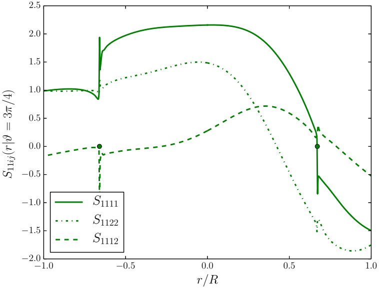


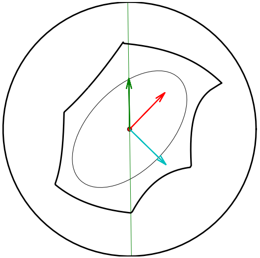


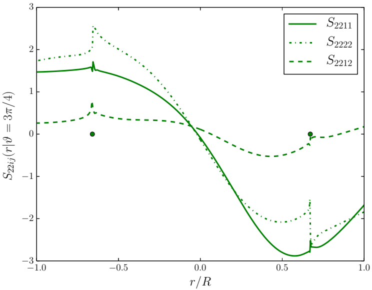


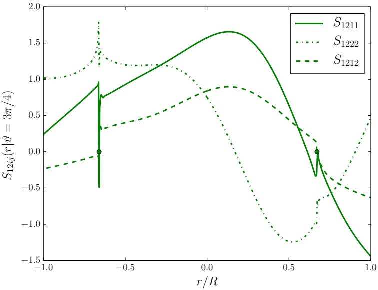
Computation of Eshelby tensor fields – Results for $\mathbb{S}(r|\vartheta)$

Projections along $\sqrt{2}/2(\underline{u}_2^\alpha - \underline{u}_1^\alpha)$ with basis $\{\underline{u}_1^\alpha, \underline{u}_2^\alpha\}$:



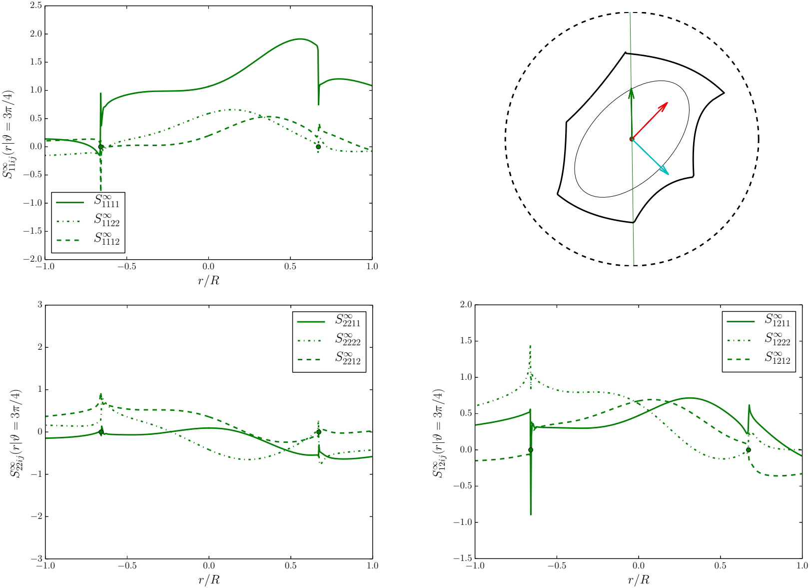






Computation of Eshelby tensor fields – Results for $\mathbb{S}^\infty(r|\vartheta)$

Projections along $\sqrt{2}/2(\underline{u}_2^\alpha - \underline{u}_1^\alpha)$ with basis $\{\underline{u}_1^\alpha, \underline{u}_2^\alpha\}$:



Stochastic simulation of disturbance fields due to random uniform eigenstrain states

We assume a random uniform eigenstrain state within $\mathcal{C}_\alpha$ given by

$$\boldsymbol{\varepsilon}^0 = \varepsilon^0 \mathbf{R}_\theta^t \cdot [\underline{u}_1^\alpha \otimes \underline{u}_1^\alpha + b\underline{u}_2^\alpha \otimes \underline{u}_2^\alpha] \cdot \mathbf{R}_\theta$$

where

$$\varepsilon^0 \sim \mathcal{U}(0, 10^{-4}) \ \ , \ \ \theta^0 \sim \mathcal{U}(0, 2\pi) \ \ , \ \ b \sim \mathcal{U}(-1, 1)$$

so that the moments of $\boldsymbol{\varepsilon}^0$ are isotropic, *i.e.* $\mathbb{E}[\boldsymbol{\varepsilon}^0] \propto \mathbf{1}$, $\mathbb{V}[\boldsymbol{\varepsilon}^0] \propto \mathbf{1}$,...

We are then interested in the field of energy density of in-plane distortion

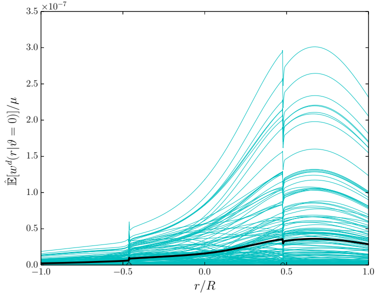
$$w^d(\underline{y}) = \mu[\boldsymbol{\varepsilon}(\underline{y}) - \mathrm{tr}(\boldsymbol{\varepsilon}(\underline{y}))\mathbf{1}/2] : [\boldsymbol{\varepsilon}(\underline{y}) - \mathrm{tr}(\boldsymbol{\varepsilon}(\underline{y}))\mathbf{1}/2]/2,$$

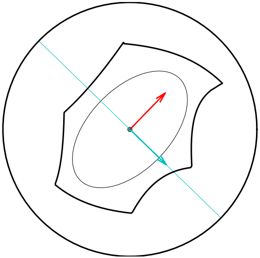
its statistical characterization and sensitivity to the morphological metrics of a random $\mathcal{C}_\alpha$.

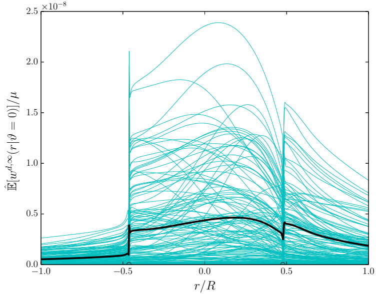
For the finite neighborhood case, estimates of the Eshelby tensor field require to specifiy a type of boundary condition (traction or displacement-free). We only consider the traction-free case, *i.e.* $\eta = -1$.

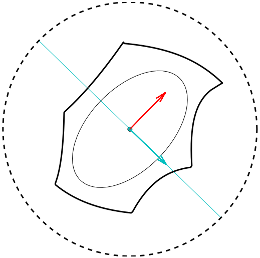
Expected in-plane distortion energy density – $\mathbb{E}[w^d(r|\vartheta)]$

Estimate from 50x50x50 realizations along $\underline{u}_1^\alpha$:



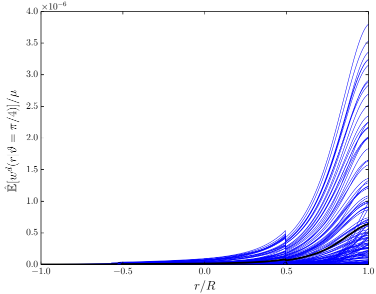


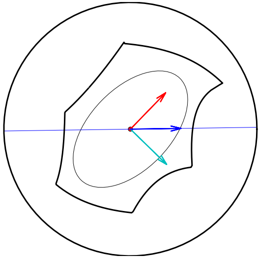


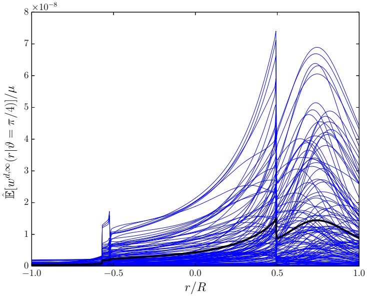


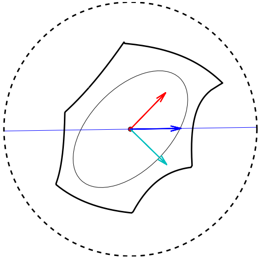
Expected in-plane distortion energy density – $\mathbb{E}[w^d(r|\vartheta)]$

Estimate from 50x50x50 realizations along $1/\sqrt{2}(\underline{u}_1^\alpha + \underline{u}_2^\alpha)$:



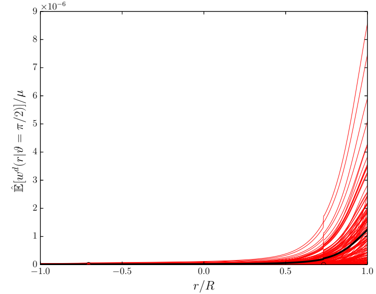


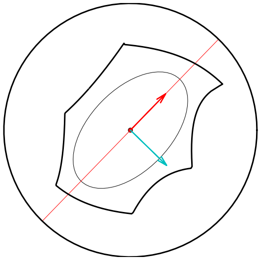


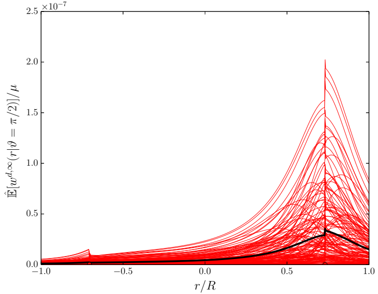


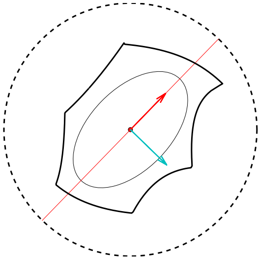
Expected in-plane distortion energy density – $\mathbb{E}[w^d(r|\vartheta)]$

Estimate from 50x50x50 realizations along $\underline{u}_2^\alpha$:



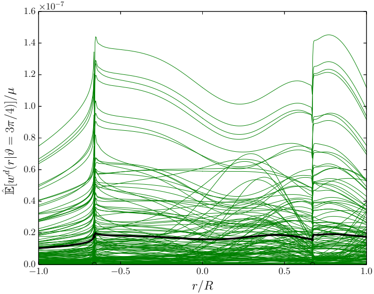


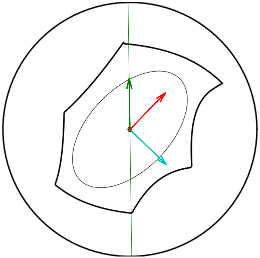


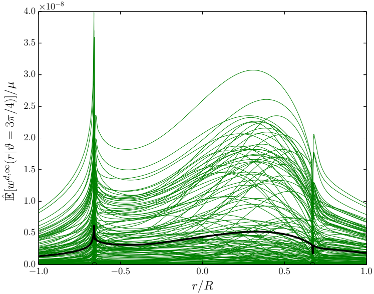


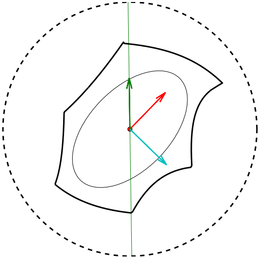
Expected in-plane distortion energy density – $\mathbb{E}[w^{d,\infty}(r|\vartheta)]$

Estimate from 50x50x50 realizations along $1/\sqrt{2}(\underline{u}_2^\alpha - \underline{u}_1^\alpha)$:

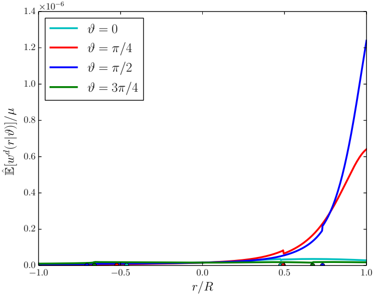


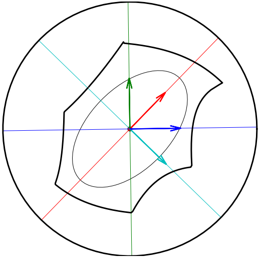


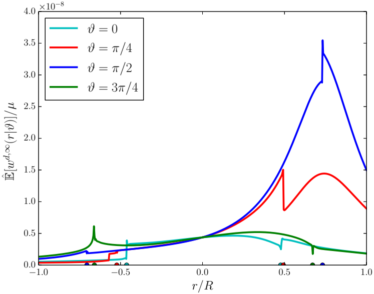


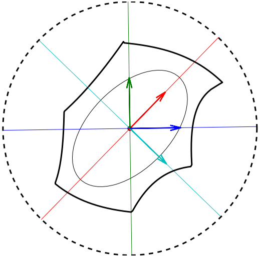


Expected in-plane distortion energy density – summary









Shape idealization for mean field and 2^{nd} order methods

Eshelbian MF methods rely on an idealization of inclusions as ellipsoids for which interior Eshelby tensors are uniform.

Question: For a given non-ellipsoidal grain $\mathcal{C}_\alpha$, what ellipsoidal idealization will minimize deviations from the actual disturbance field?

At first, $\langle \mathbb{S}^\infty(\underline{y}) \rangle_{\mathcal{C}_\alpha}$ may seem to be a good estimate

$$\tilde{\Delta} \equiv \sqrt{\frac{\langle [\mathbb{S}^\infty(\underline{y}) - \langle \mathbb{S}^\infty(\underline{y}) \rangle_{\mathcal{C}_\alpha}] :: [\mathbb{S}^\infty(\underline{y}) - \langle \mathbb{S}^\infty(\underline{y}) \rangle_{\mathcal{C}_\alpha}] \rangle_{\mathcal{C}_\alpha}}{\langle \mathbb{S}^\infty(\underline{y}) \rangle_{\mathcal{C}_\alpha} :: \langle \mathbb{S}^\infty(\underline{y}) \rangle_{\mathcal{C}_\alpha}}}$$

but for arbitrary $\mathcal{C}_\alpha$, $\langle \mathbb{S}^\infty(\underline{y}) \rangle_{\mathcal{C}_\alpha}$ is less symmetric than the Eshelby tensor of an ellipsoid. Alternatively, we consider ellipsoids of 2nd order Minkowski tensors

$$\Delta_\nu^{\infty,r,s} \equiv \sqrt{\frac{\langle [\mathbb{S}^\infty(\underline{y}) - \mathbb{S}_\nu^{\infty,r,s}] :: [\mathbb{S}^\infty(\underline{y}) - \mathbb{S}_\nu^{\infty,r,s}] \rangle_{\mathcal{C}_\alpha}}{\mathbb{S}_\nu^{\infty,r,s} :: \mathbb{S}_\nu^{\infty,r,s}}}$$

To do: Investigate $\Delta_\nu^{\infty,r,s}$ for arbitrary Poisson's ratios and identify the best fitting 2nd order Minkowski tensor ellipsoid.

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$$\Delta(\langle \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha}, \mathcal{E}) = \sqrt{\frac{[\langle \boldsymbol{\varepsilon} \rangle_{\mathcal{E}} - \langle \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha}] : [\langle \boldsymbol{\varepsilon} \rangle_{\mathcal{E}} - \langle \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha}]}{\langle \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha} : \langle \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha}}}$$

but for arbitrary $\mathcal{C}_\alpha$, $\langle \mathbb{S}^\infty(\underline{y}) \rangle_{\mathcal{C}_\alpha}$ is less symmetric than the Eshelby tensor of an ellipsoid. Alternatively, we consider ellipsoids of 2nd order Minkowski tensors

$$\Delta(\langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha}, \mathcal{E}) = \sqrt{\frac{[\langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\mathcal{E}} - \langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha}] :: [\langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\mathcal{E}} - \langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha}]}{\langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha} :: \langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\mathcal{C}_\alpha}}}$$

To do: Investigate $\Delta_\nu^{\infty,r,s}$ for arbitrary Poisson's ratios and identify the best fitting 2nd order Minkowski tensor ellipsoid.

Effect of shape idealization on nonlinear homogenization

Whether they use Eshelby tensors or not, most of the nonlinear homogenization scheme rely on ellipsoidal shape idealization:

- Affine procedures (AFF): Zaoui and Masson (1998), Masson et al. (2000)
- Transformation field analysis (TFA): Dvorak and Rao (1976), Dvorak et al. (1988), Dvorak and Benveniste (1992)
- Generalized transformation field analysis: Michel and Suquet (1997), Moulinec and Suquet (1998)
- Nonlinear Hashin-Shtrikman-based approach: Michel and Suquet (1997), Moulinec and Suquet (1998)
- Optimized linear comparison composites (LCC): Ponte-Castaneda (1991), Suquet (1993)
- 2nd order comparison composites: Ponte-Castaneda (1996), Suquet and Ponte-Castaneda (1993),

Question: For a given non-ellipsoidal grain $\mathcal{C}_\alpha$, what ellipsoidal idealization will minimize the deviations of homogenization-based predictions from full-field-based predicted?

Questions/Comments

Sensitivity analysis of energy distortion fluctuations to morphological characteristics of random grains

For this simple mechanical problem, we want to understand what *types* and *orders* of morphological metrics of a random grain $\mathcal{C}_\alpha$ plays a significant role on localization.

We define measures of fluctuation of energy distortion such as:

$$\langle \mathbb{E}[w^d(\underline{y})] - \langle \mathbb{E}[w^d(\underline{y})] \rangle_{\mathcal{C}_\alpha} \rangle_{\mathcal{C}_\alpha} \quad \text{and} \quad \langle \mathbb{E}[w^d(\underline{y})] - \langle \mathbb{E}[w^d(\underline{y})] \rangle_{\underline{\mathcal{C}}_\alpha} \rangle_{\underline{\mathcal{C}}_\alpha}$$
$$\langle (\mathbb{E}[w^d(\underline{y})] - \langle \mathbb{E}[w^d(\underline{y})] \rangle_{\mathcal{C}_\alpha})^2 \rangle_{\mathcal{C}_\alpha} \quad \text{and} \quad \langle (\mathbb{E}[w^d(\underline{y})] - \langle \mathbb{E}[w^d(\underline{y})] \rangle_{\underline{\mathcal{C}}_\alpha})^2 \rangle_{\underline{\mathcal{C}}_\alpha}$$

where $\underline{\mathcal{C}}_\alpha = B(\underline{x}_\alpha, R) \setminus \mathcal{C}_\alpha$ to quantify localization outside and within a grain subjected to a uniform eigenstrain.

Then, we simulate realizations of random grains $\mathcal{C}_\alpha$ and we investigate correlations with W_0/R^2, W_1/R, $W_2 R$, $I_2(\mathbf{W}_0^{2,0})/R^4$, $I_2(\mathbf{W}_1^{2,0})/R^2$, $I_2(\mathbf{W}_1^{2,0})R^2$, ...