Stochastic Simulation of Random Material Microstructures using Ellipsoidal Growth Structures (EGS)

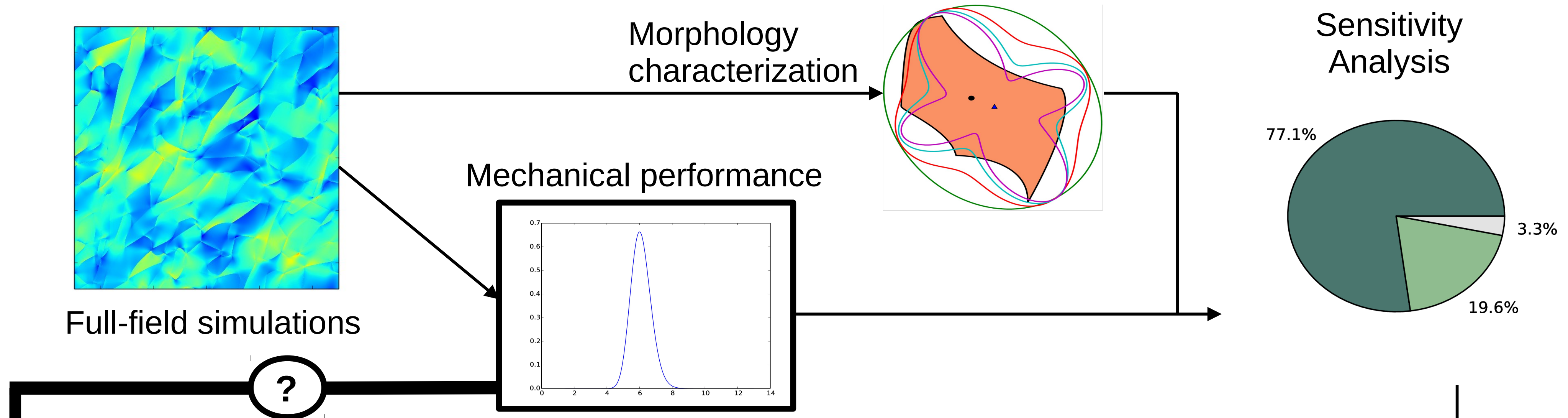
N. Venkovic
nvenkov1@jhu.edu

L. Graham-Brady
lori@jhu.edu

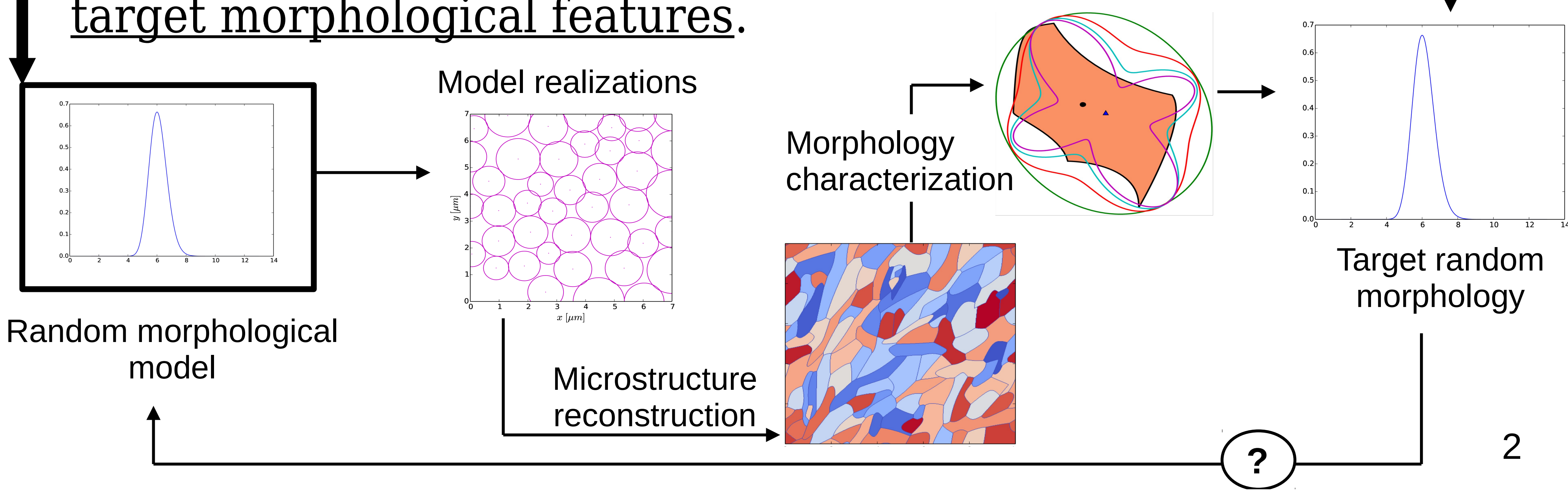
EMI/PMC
May 25, 2016

Motivation/Objective

- Identify relevant and sufficient morphological metrics for the prediction of specific mechanical performances.



- Simulate random instances of material microstructures with target morphological features.



Outline

- Ellipsoidal growth structures (EGS)
  - Definition
  - Resolution
  - Simulation

- Morphological characterization of single cells
  - Minkowski tensors – Expressions
  - Results

- Mechanical systems of interest
  - Eshelby tensor fields of EGS cells

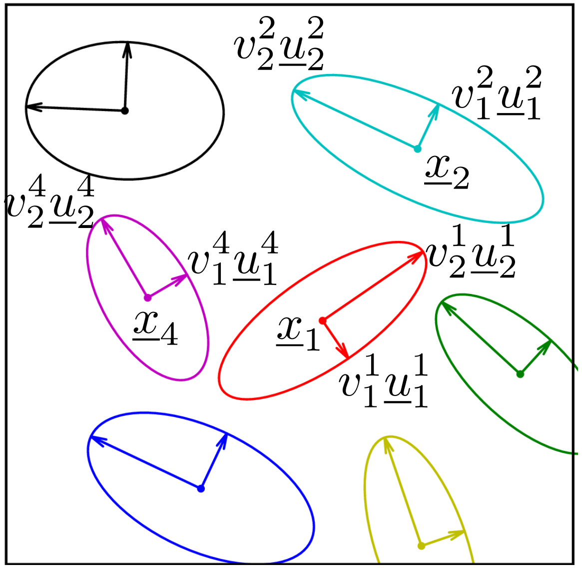
Ellipsoidal growth structures (EGS)

Ellipsoidal growth structures (EGS) are morphological models defined with marked point patterns (MPP). Underlying microstructures are constructed after a rule invoking the MPP.

Example: Tessellations.

- MPP: $\{(\underline{x}_\alpha, \mathbf{Z}_\alpha)\}$
- Rule: $\Omega_\alpha = \{\underline{x} \,|\operatorname*{argmin}_\gamma (\underline{x} - \underline{x}_\gamma) \cdot \mathbf{Z}_\gamma \cdot (\underline{x} - \underline{x}_\gamma) = \alpha\}$

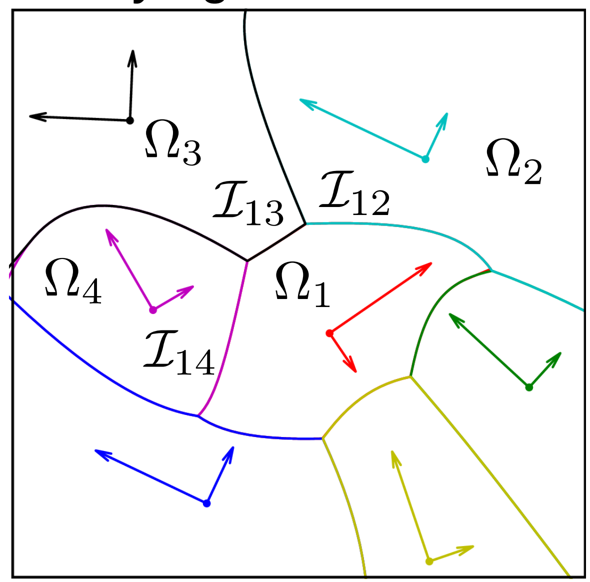
MPP



$$\mathbf{Z}_\alpha = \frac{\underline{u}_1^\alpha \otimes \underline{u}_1^\alpha}{(v_1^\alpha)^2} + \frac{\underline{u}_2^\alpha \otimes \underline{u}_2^\alpha}{(v_2^\alpha)^2}$$

Resolution

Underlying microstructure



Every cell Ω_α with boundary $\partial\Omega_\alpha$ can be reconstructed from common curves $\mathcal{I}_{\alpha\gamma}$. Can we solve for $\mathcal{I}_{\alpha\gamma}$?

EGS – Transformation

Solving for parameterizations of common curves $\mathcal{I}_{\alpha\gamma}$ is difficult. To circumvent this difficulty, we introduce a diffeomorphic transformation.

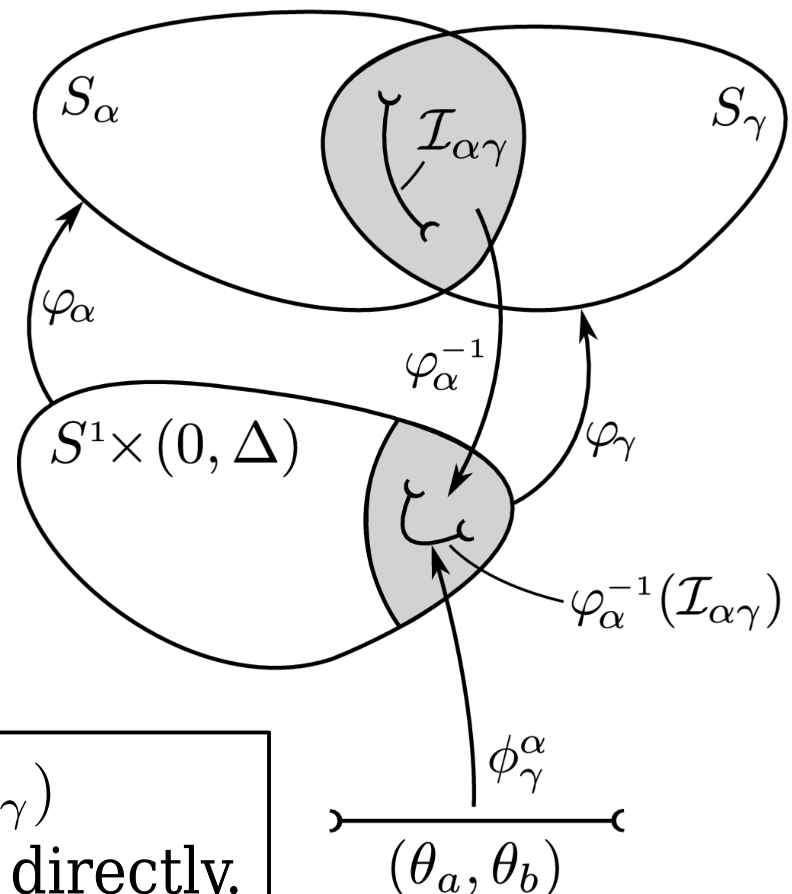
Let every point of a growing ellipse be given by a time-dependent mapping from a unit circle:

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

We let the common curves be

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

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

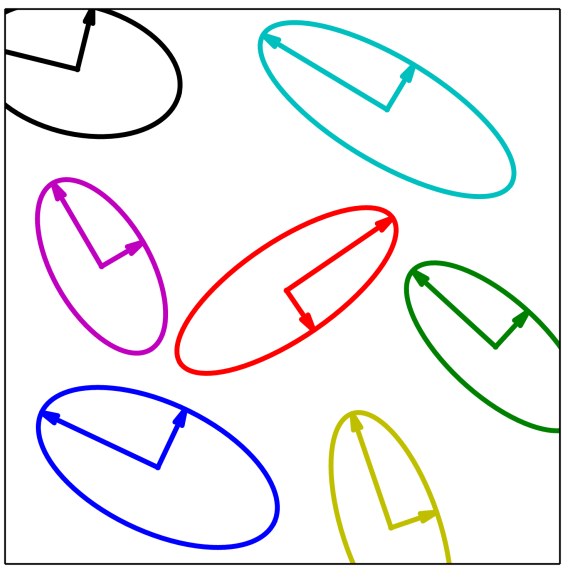


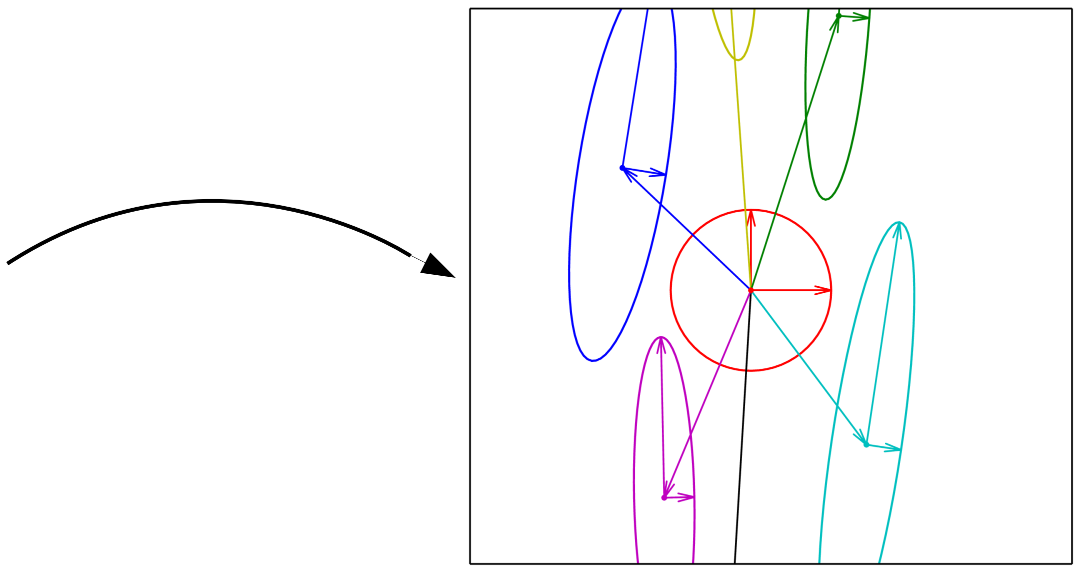
Finding parameterizations ϕ_γ^α of $\varphi_\alpha^{-1}(\mathcal{I}_{\alpha\gamma})$ is much easier than parameterizing $\mathcal{I}_{\alpha\gamma}$ directly.

EGS – Transformation (illustration)

Solving for charts ϕ_γ^α is equivalent to solve for times at which a given point in S^1 is intersected by a moving ellipse of fixed dimensions.

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





Contact function:

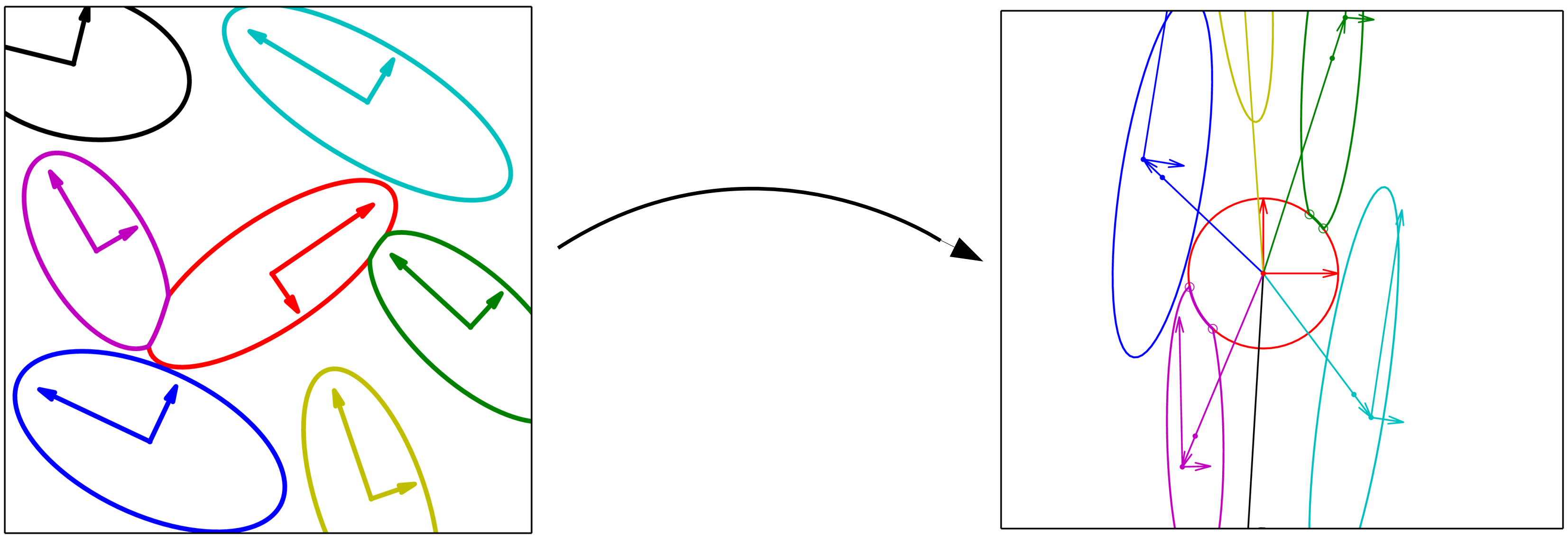
$$\xi_\gamma^\alpha = \frac{\underline{x}_\gamma^\alpha \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha}{\underline{x}(\theta) \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha + \delta\sqrt{\left(\underline{x}(\theta) \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha\right)^2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

Still, common points (locations of triple junctions) must be solved numerically.

EGS – Transformation (illustration)

Solving for charts ϕ_γ^α is equivalent to solve for times at which a given point in S^1 is intersected by a moving ellipse of fixed dimensions.

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



Contact function:

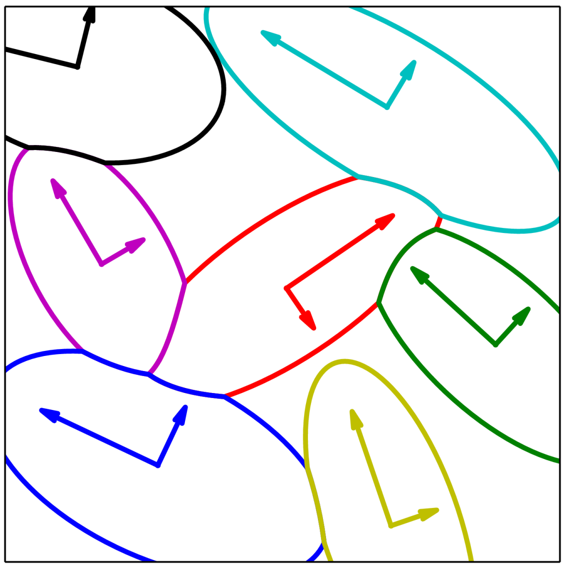
$$\xi_\gamma^\alpha = \frac{\underline{x}_\gamma^\alpha \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha}{\underline{x}(\theta) \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha + \delta \sqrt{\left(\underline{x}(\theta) \cdot \mathbf{Z}_\gamma^\alpha \cdot \underline{x}_\gamma^\alpha\right)^2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

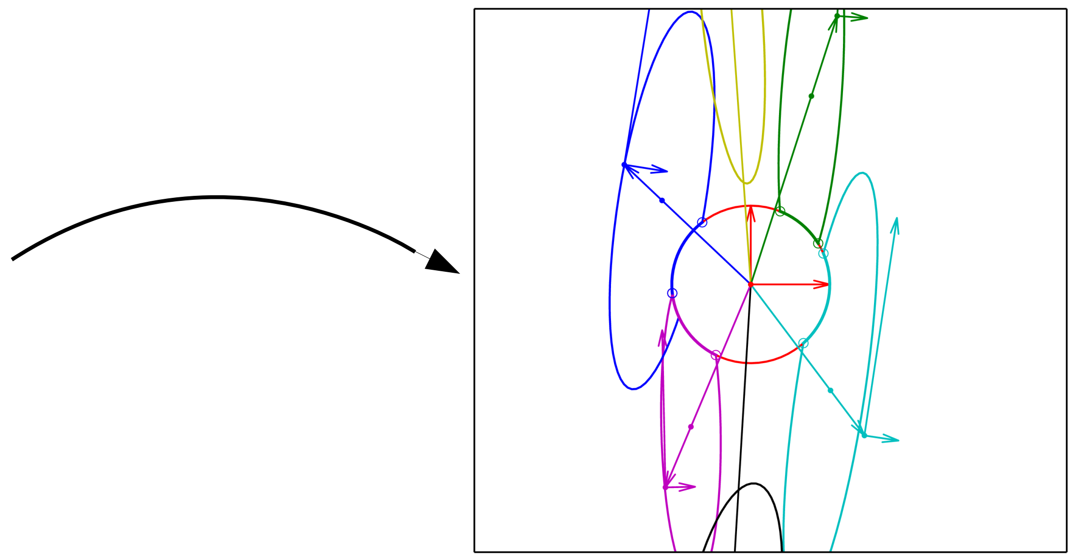
Still, common points (locations of triple junctions) must be solved numerically.

EGS – Transformation (illustration)

Solving for charts ϕ_γ^α is equivalent to solve for times at which a given point in S^1 is intersected by a moving ellipse of fixed dimensions.

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





Contact function:

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

Still, common points (locations of triple junctions) must be solved numerically.

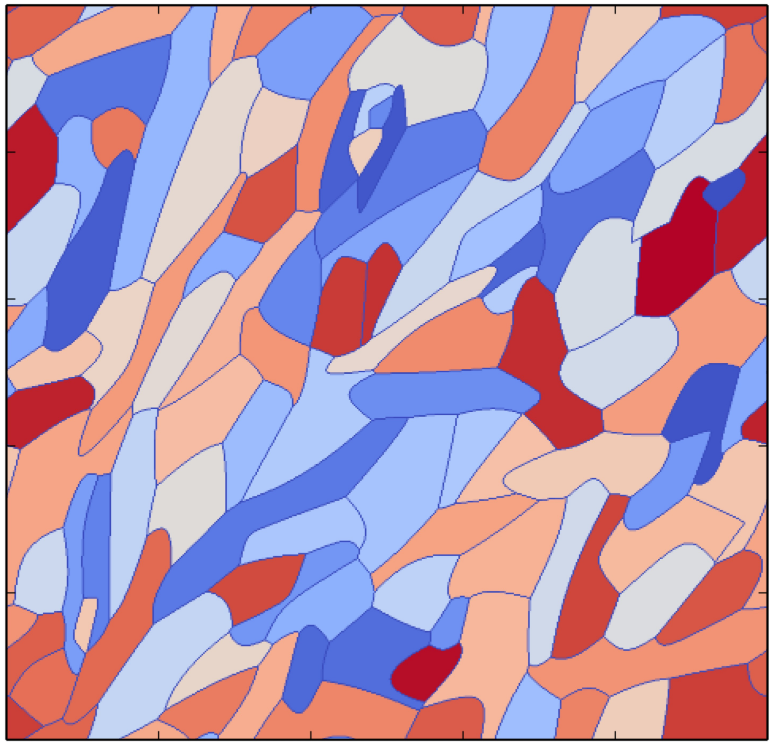
EGS – Types of microstructures

For the same definition of common curves, i.e. f_γ^α , we try to generate different types of underlying microstructures by changing the contact functions.

Space filling models (Tess.):

$$\xi_\gamma^\alpha = \tilde{\xi}_\gamma^\alpha$$

(1 common curve per pair of neighbors)



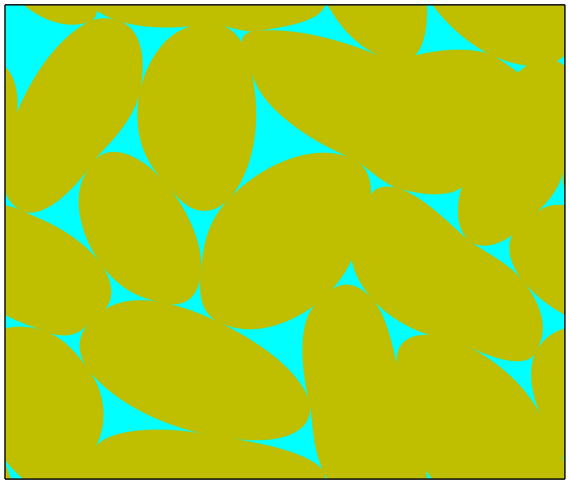
Non-space filling models:

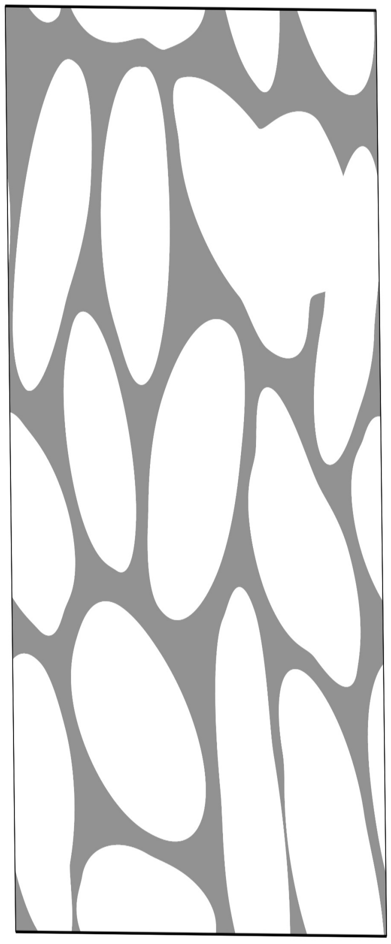
$$\xi_\gamma^\alpha \leq \tilde{\xi}_\gamma^\alpha$$

$$\downarrow$$

$$\mathcal{I}_{\alpha\gamma} \neq \mathcal{I}_{\gamma\alpha}$$

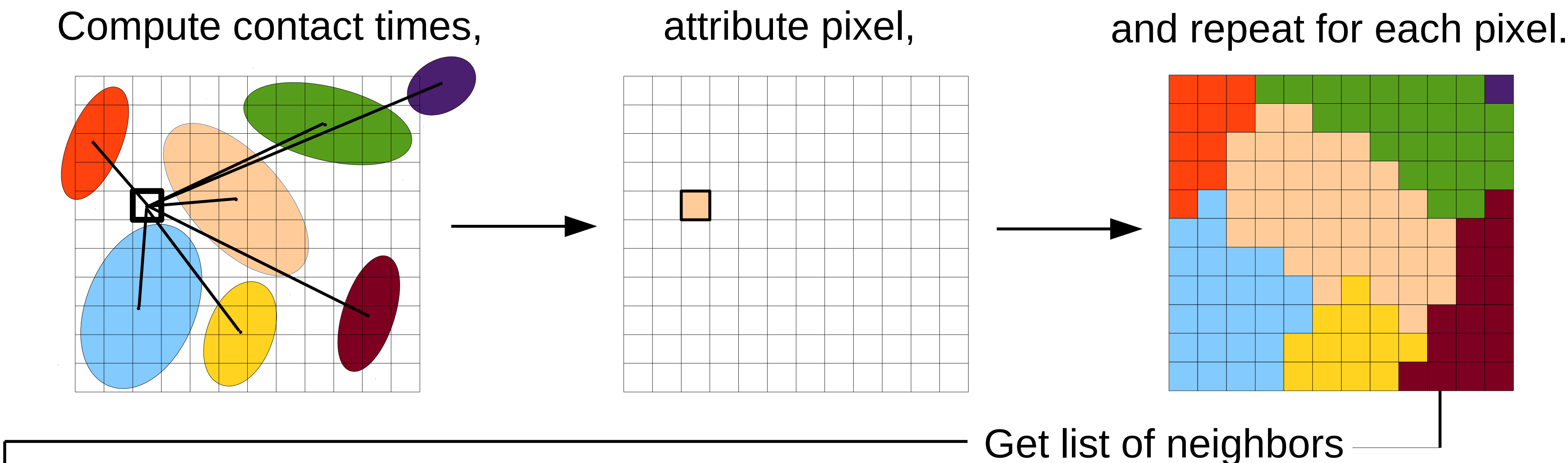
(2 common curves per pair of neighbors)



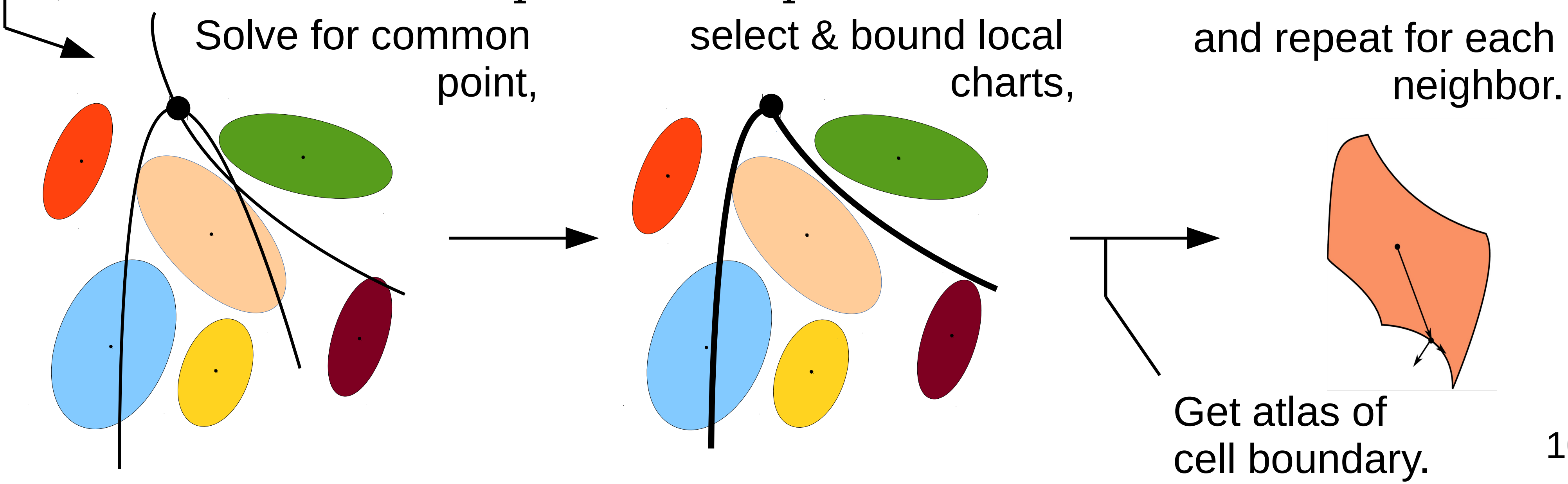


EGS – Resolution

I) Discretize and solve numerically for lists of neighbors.



II) Solve for common points with parameterizations of common curves.



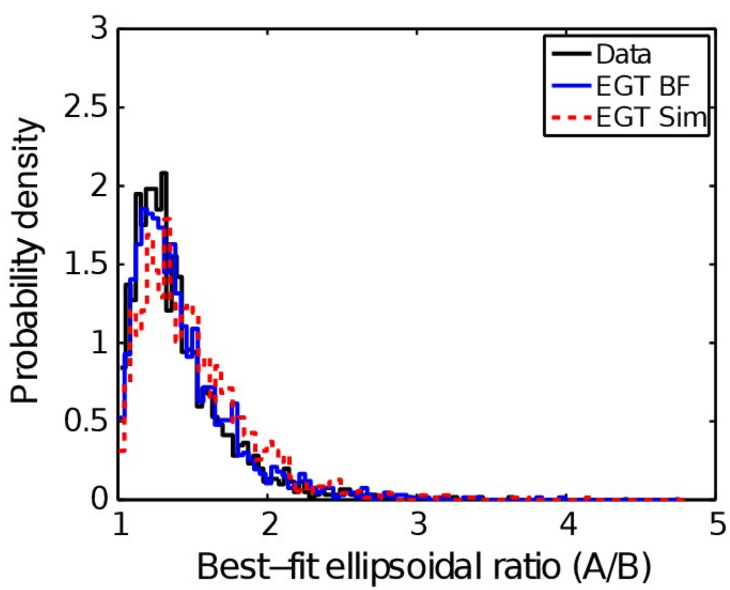
EGS – Simulation

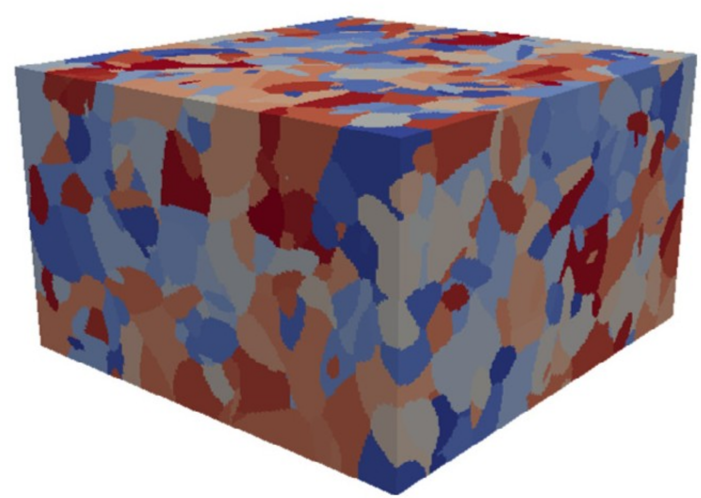
For random materials, EGS can be interpreted as realizations of a marked point process $\{(\underline{\xi}, m_{\xi}), \underline{x} \in \Xi, m_{\xi} \in M\}$ with marks $m_{\xi} = \{v_1, v_2, \theta\}$

Realizations can be drawn by:

- 1) Simulating a (hard-core) point process,
- 2) Simulating the marks after a conditional distribution on the nucleation sites.

Teferra and Graham-Brady (2015): Realizations of polycrystalline microstructures can be obtained considering no correlation of marks between sites (cells) that reproduce size and inertial aspect ratios:

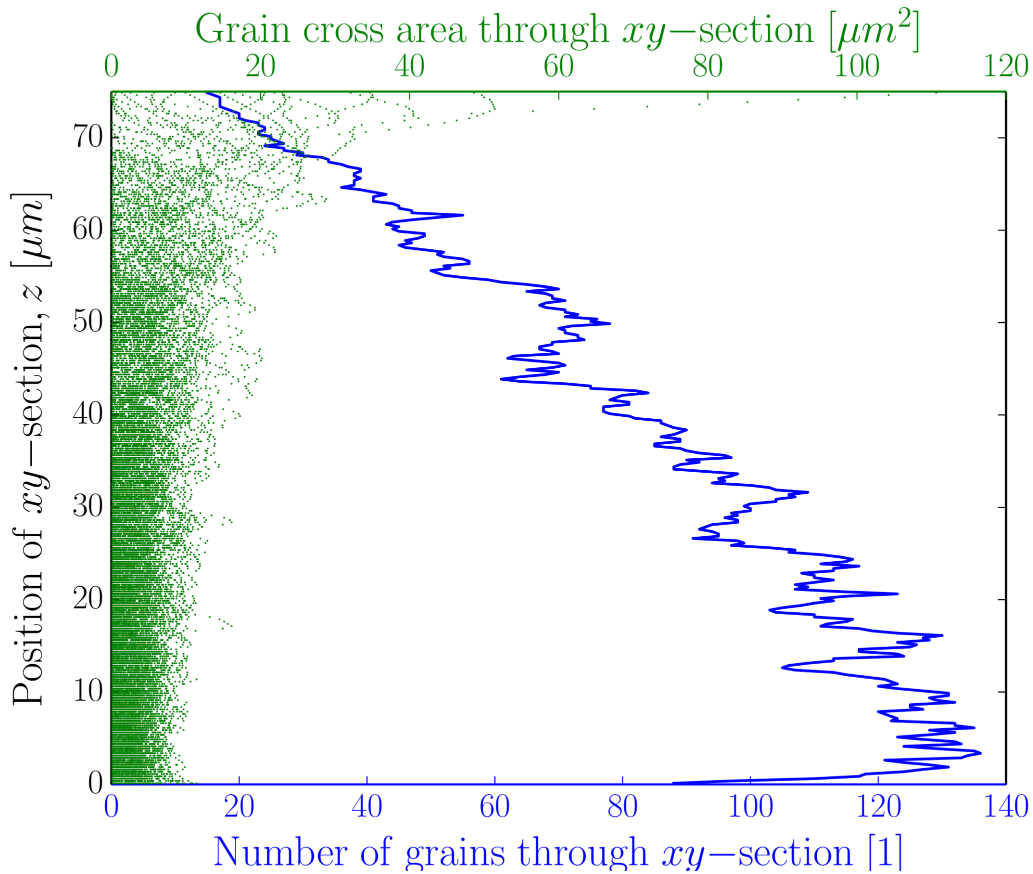




EGS – Simulation

However, for the purpose of simulation, the point process does not need to be stationary.

Realization of a non-stationary process / Functionally graded microstructure:

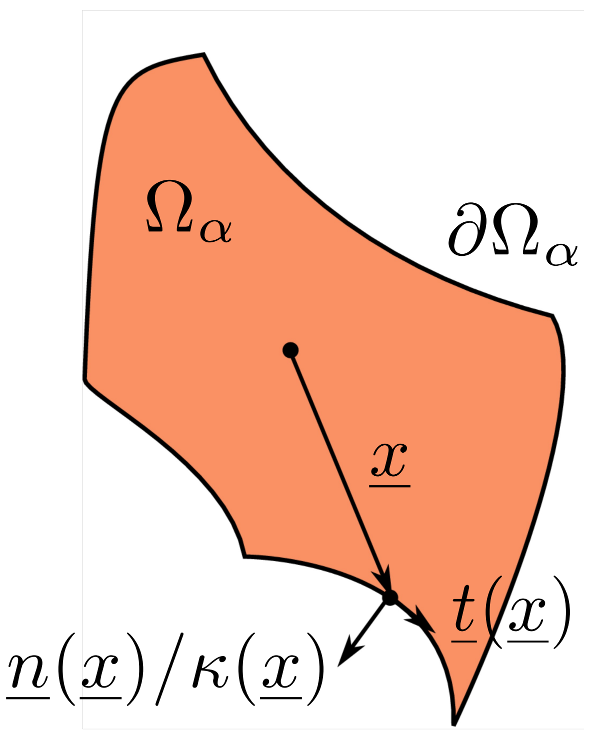


Single grain morphology characterization

Single grains are characterized using Minkowski tensors:

Measures of mass distribution:

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

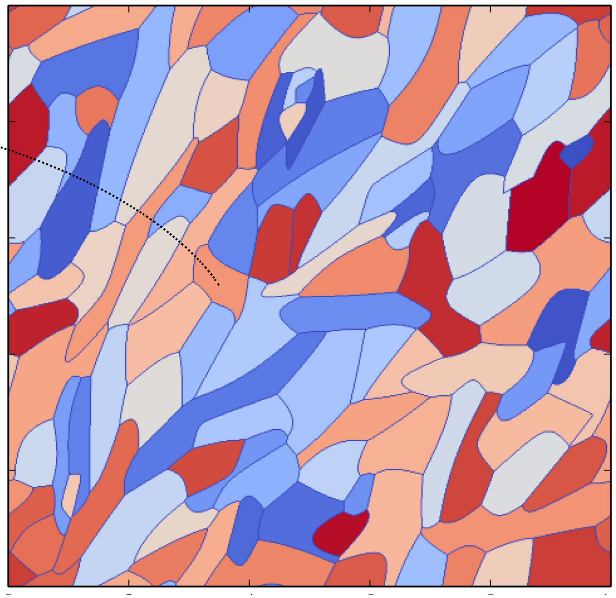


Measures of surface distribution:

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

Curvature-weighted measures of surface distribution:

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



Expressions of Minkowski tensors for EGS

Using the parameterization of the EGS, the following expressions are obtained:

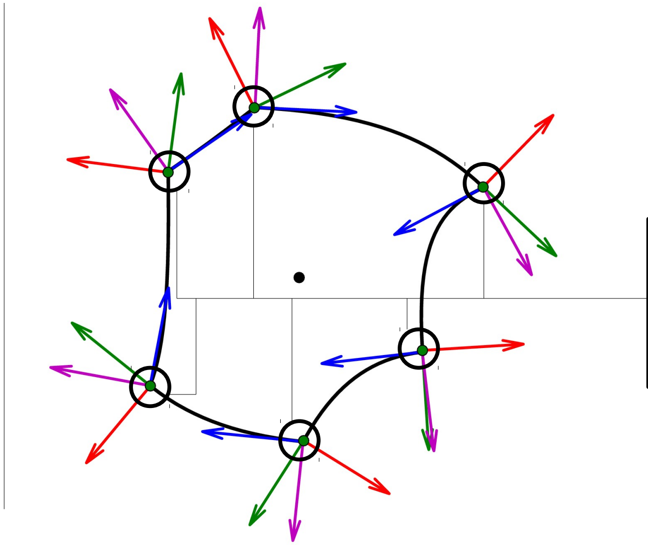
$\underline{x}_\alpha$, $\underline{u}_1^\alpha$ and $\underline{u}_2^\alpha$ are from the MPP.

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

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

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

where $I_0^{i,j}$ and $I_\nu^{i,j,k,l}$ are scalar coefficients obtained by integration of the locally defined contact functions ξ.



Effect of common points

Expressions of Minkowski tensors for EGS

Interdependences between different metrics allow us to reduce the number of integrals to compute:

Because $\partial\mathcal{C}_\alpha$ is closed, $\underline{W}_1^{0,1} = \underline{0}$ and $I_1^{0,0,0,1} = I_1^{0,0,1,0} = 0$.

From $\mathbf{W}_1^{1,1} = W_1 \mathbf{1}$ we find $I_1^{1,0,1,0} = I_1^{0,1,0,1} = 0$,

and $I_1^{0,1,1,0} = I_1^{1,0,0,1} = I_0^{0,0}$.

From $\sum_{i_k=1}^{2} \dots \sum_{i_2=1}^{2} \sum_{i_1=1}^{2} \underline{u}_{i_k}^{\alpha^{\otimes 2}} : \left[\dots \underline{u}_{i_2}^{\alpha^{\otimes 2}} : \left[\underline{u}_{i_1}^{\alpha^{\otimes 2}} : \mathcal{W}_1^{0,2k} \right] \dots \right] = W_1$ →

$$\sum_{\ell=0}^{k} \binom{k}{\ell} I_1^{0,0,2\ell,2(k-\ell)} = I_1^{0,0,0,0}$$

From

$$\sum_{i_k=1}^{2} \dots \sum_{i_2=1}^{2} \sum_{i_1=1}^{2} \underline{u}_{i_k}^{\alpha^{\otimes 2}} : \left[\dots \underline{u}_{i_2}^{\alpha^{\otimes 2}} : \left[\underline{u}_{i_1}^{\alpha^{\otimes 2}} : \mathcal{W}_1^{0,2k+1} \right] \dots \right] = \underline{W}_1^{0,1}$$ →

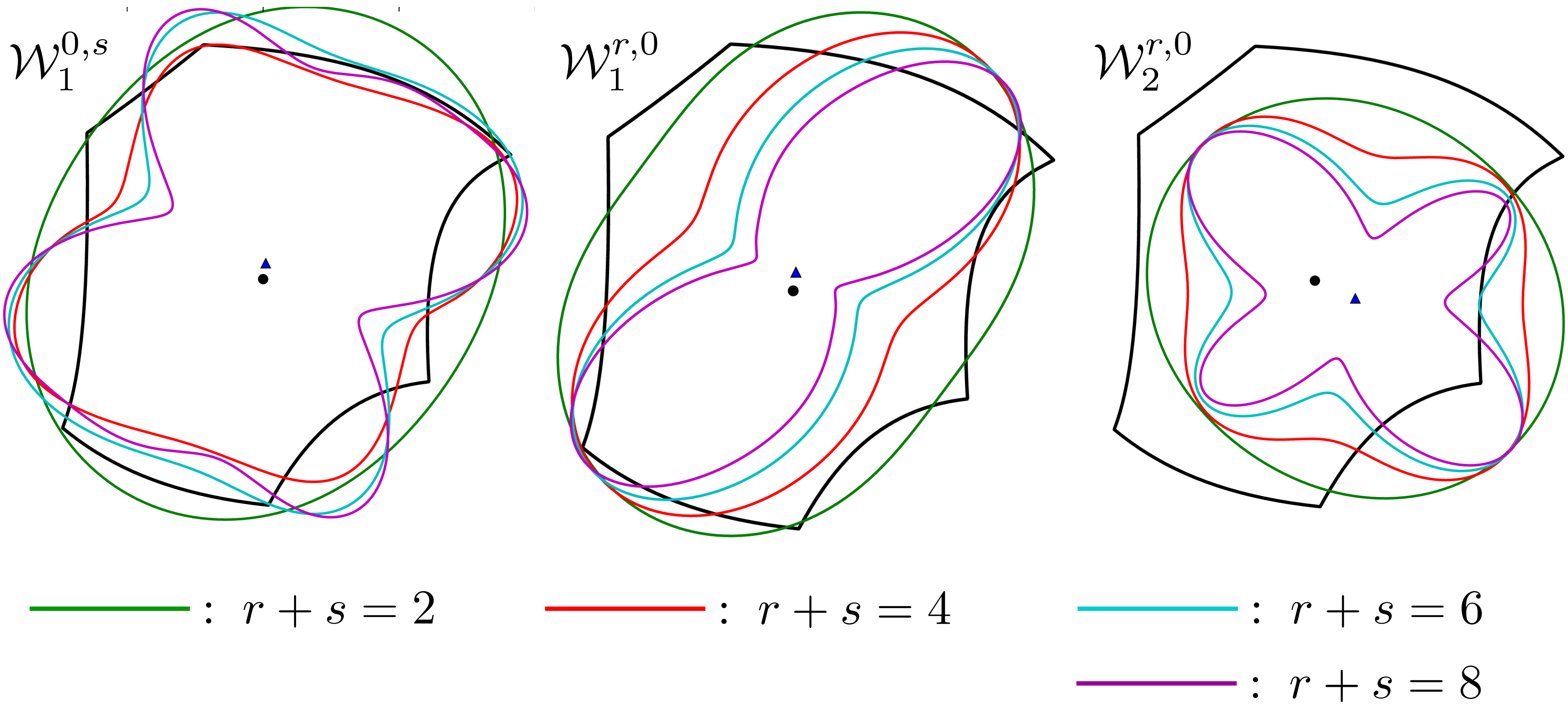
$$\sum_{\ell=0}^{k} \binom{k}{\ell} I_1^{0,0,2\ell,2(k-\ell)+1} = \sum_{\ell=0}^{k} \binom{k}{\ell} I_1^{0,0,2(k-\ell)+1,2\ell} = 0$$

Similarly,

$$\sum_{\ell=0}^{k} \binom{k}{\ell} I_1^{0,0,2\ell,2(k-\ell+1)} = I_1^{0,0,0,2}, \sum_{\ell=0}^{k} \binom{k}{\ell} I_1^{0,0,2(k-\ell+1),2\ell} = I_1^{0,0,2,0}$$ and so on ...

Minkowski tensors – Results

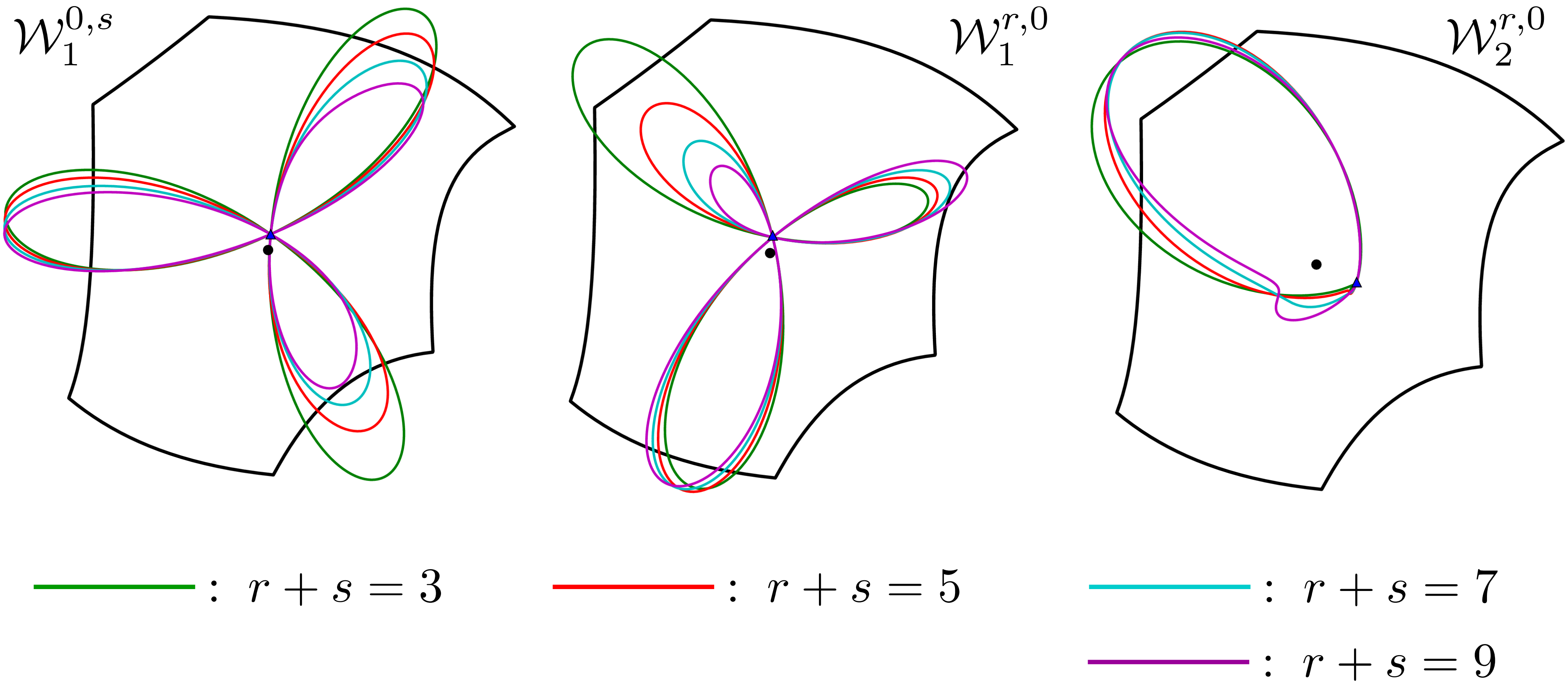
Normalized radial projections of some even-ordered metrics:



What types and orders of Minkowski tensors are sufficient metrics for a grain? What about “mixed orders”?

Minkowski tensors – Results

Normalized radial projections of some odd-ordered metrics:



We would like to understand which of these can be used to predict mechanical behaviors.

Mechanical systems under study

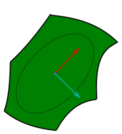
#1 Isotropic Eshelby problem

- Response of the system almost entirely limited to morphology (and Kolosov's constant),

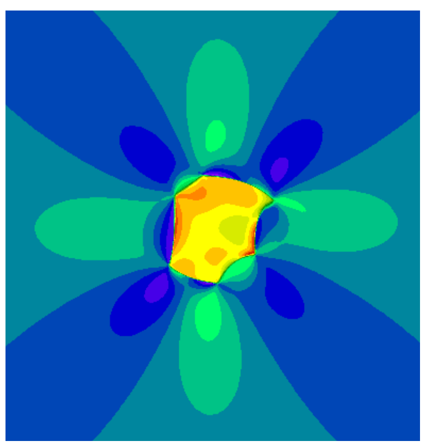
- No effect of neighbors.

- Can we relate Hill (or Eshelby) tensor fields to the Minkowski tensors?

$$\boldsymbol{\varepsilon}^0 = \varepsilon^0_{12} \underline{e}_1 \overset{s}{\otimes} \underline{e}_2$$



$$\varepsilon_{12}(\underline{x})$$



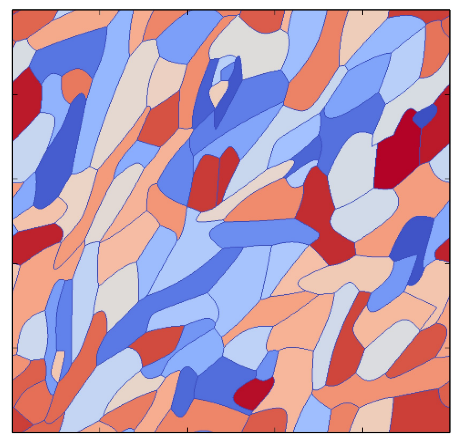
#2 Elastic behavior of periodic anisotropic polycrystals

- Effect of neighboring grain morphology,

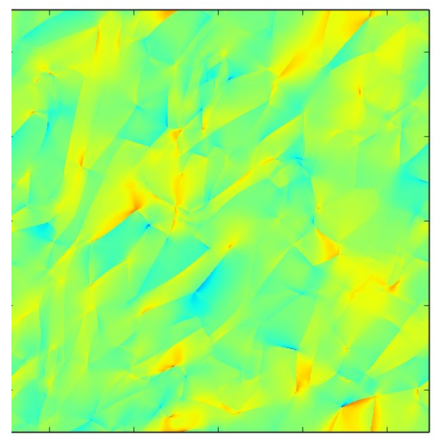
- Effect of lattice mis-orientations.

- Can we understand how stiffness and morphology interact for the localization of elastic fields?

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



$$\varepsilon_{22}(\underline{x})$$



Eshelby tensor fields for EGS cells

Using the parameterizations of the cell boundaries, expressions for the unbounded (and bounded, not here) Eshelby tensor fields can be recovered in terms of the marks of the MPP.

Using the irreducible representation by Zheng et al. (2007):

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

From MPP

with $\mathbf{d}(\underline{y}) = \Re\{\gamma_2(\underline{y})\}\Re\{(\underline{u}_1^{\alpha} + i\underline{u}_2^{\alpha})^{\otimes^2}\} + \Im\{\gamma_2(\underline{y})\}\Im\{(\underline{u}_1^{\alpha} + i\underline{u}_2^{\alpha})^{\otimes^2}\}$

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

and

Related to morphology only

$$\boxed{\gamma_2(\underline{y})} = \frac{1}{4\pi i}\int_{\pi\circ\varphi_{\alpha}^{-1}(\partial\mathcal{C}_{\alpha})} \frac{\partial_{\theta}[\xi(\theta)\underline{x}(\theta)] \cdot \mathbf{Z}_{\alpha}^{-1/2} \cdot (\underline{u}_1^{\alpha} + i\underline{u}_2^{\alpha})}{[\underline{x}_{\alpha} + \xi(\theta)\mathbf{Z}_{\alpha}^{-1/2} \cdot \underline{x}(\theta) - \underline{y}] \cdot (\underline{u}_1^{\alpha} - i\underline{u}_2^{\alpha})}\mathrm{d}\theta$$

$$\boxed{\gamma_4(\underline{y})} = \frac{1}{4\pi i}\int_{\pi\circ\varphi_{\alpha}^{-1}(\partial\mathcal{C}_{\alpha})} \frac{\{[\underline{x}_{\alpha} + \xi(\theta)\mathbf{Z}_{\alpha}^{-1/2} \cdot \underline{x}(\theta) - \underline{y}] \otimes \partial_{\theta}[\xi(\theta)\underline{x}(\theta)] \cdot \mathbf{Z}_{\alpha}^{-1/2}\} : (\underline{u}_1^{\alpha} + i\underline{u}_2^{\alpha})^{\otimes^2}}{[\underline{x}_{\alpha} + \xi(\theta)\mathbf{Z}_{\alpha}^{-1/2} \cdot \underline{x}(\theta) - \underline{y}] \cdot (\underline{u}_1^{\alpha} - i\underline{u}_2^{\alpha})}\mathrm{d}\theta$$

Conclusion

- Morphological models are being developed for different types of material microstructures,
- Parameterizations are obtained for the underlying microstructures of these models,
- Exhaustive characterization of morphologies is performed using these parameterizations,
- Correlations between these morphological metrics and the localization of elastic fields is being investigated.
- Next steps:
  - Complete sensitivity analysis of mechanical performance to morphological metrics,
  - Identify relevant metrics and target distributions,
  - Investigate plastic behaviors,
  - Perform backward analysis for identification of underlying morphological models.