Stochastic morphological simulation based on partial statistical description of polycrystals

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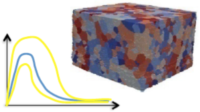
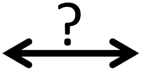
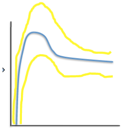
Structure - Property Relation







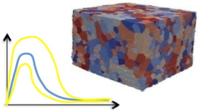
- Grain size, shape, boundary type
- Crystallographic orientation
- Phase configuration

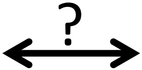
- Dissipation mechanism
- Strength, ductility
- Thermal, electrical conductivity

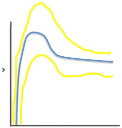
Objective: Facilitate the development of a better understanding of the mechanical behavior of polycrystals by means of numerical simulation.

Motivation, Objective and Approach

Structure - Property Relation







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Microstructure simulation

Approach: Enable the simulation of polycrystalline microstructures with target:

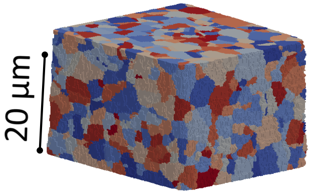
- Distribution of morphological features;
- and correlation structures.

Parameterization of polycrystalline microstructures

Polycrystalline microstructures are generally represented as digitalized data sets; for instance this sample of nickel super-alloy IN100

Data set from EBSD:

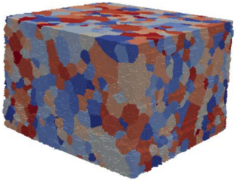
- Data consuming;
- Finite resolution.



4, 444, 713 parameters

Parameterization by ellispoidal growth tessellation

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



14, 118 parameters

Presentation outline

1. Ellipsoidal growth tessellation: a model for morphologically anisotropic polycrystals.
2. Tessellation resolution: from numerical to semi-analytical solutions.
3. Transformation of the problem: from growth to collision.
4. Grain boundary resolution: a semi-analytical approach.
5. Morphology characterization: using Minkowski valuations.
6. Stochastic simulation with target morphological features: next steps and objectives.

Ellipsoidal growth tessellation (EGT) — Definition

- Tessellation on $\mathbb{R}^d$: *Countable* set $m = \{\mathring{\mathcal{C}}_\alpha\}$ of *disjoint* and *space-filling* cells $\mathring{\mathcal{C}}_\alpha \subset \mathbb{R}^d$:

$$\mathring{\mathcal{C}}_\alpha \cap \mathring{\mathcal{C}}_\gamma = \emptyset \quad ; \quad \bigcup_\alpha \mathring{\mathcal{C}}_\alpha = \mathbb{R}^d \quad ; \quad \#\{\mathring{\mathcal{C}}_\alpha \cap m \,|\, \mathring{\mathcal{C}}_\alpha \cap \mathcal{B} \neq \emptyset\} < \infty \; \forall \, \mathcal{B} \subset \mathbb{R}^d$$

- Multiplicatively weighted anisotropic Voronoi tessellation:

$$\mathcal{C}_\alpha = \{\underline{x} \in \mathbb{R}^d \,|\, T_\alpha(\underline{x}) < T_\gamma(\underline{x}) \; \forall \, \gamma \neq \alpha\}$$

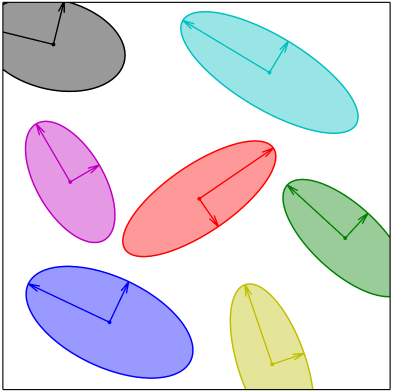
where $T_\alpha(\underline{x}) \equiv (\underline{x} - \underline{x}^\alpha) \cdot \mathbf{Z}_\alpha \cdot (\underline{x} - \underline{x}^\alpha)$ and

$$\mathbf{Z}_\alpha = \sum_{j=1}^{d} \frac{\underline{u}_j^\alpha \otimes \underline{u}_j^\alpha}{(v_j^\alpha)^2}$$

while $\underline{u}_j^\alpha \in \mathbb{R}^d$ and $v_j^\alpha \in \mathbb{R}^+$ such that every $\mathbf{Z}_\alpha$ is a second-rank positive definite tensor.

Ellipsoidal growth tessellation (EGT) — Definition

- Grain growth analogy: Every tensor $\mathbf{Z}_\alpha^{-1/2}$ is a representation of an ellipsoidal velocity profile with principal component v_j^α along $\underline{u}_j^\alpha$.



- For a cell with velocity profile $\mathbf{Z}_\alpha^{-1/2}$ growing from $\underline{x}_\alpha$:
  - $T_\alpha(\underline{x})$ is the time necessary for the cell to reach $\underline{x}$;
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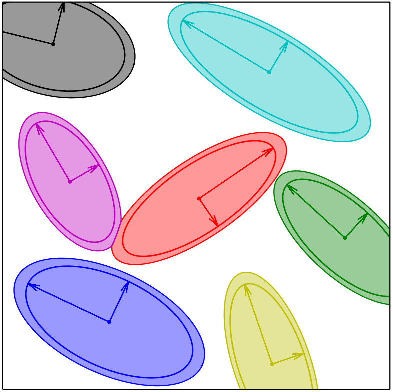

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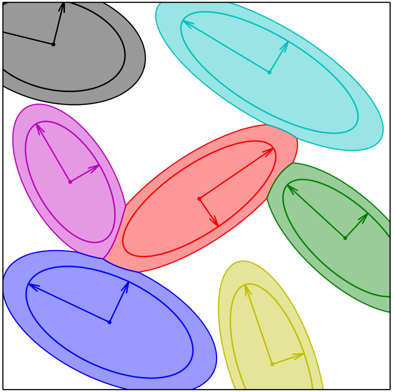

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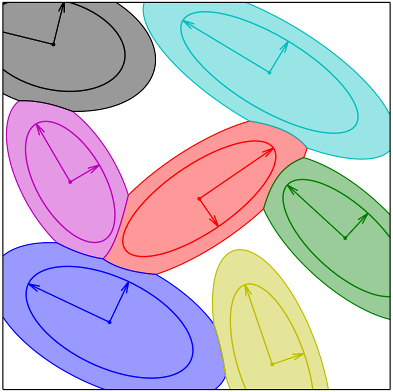

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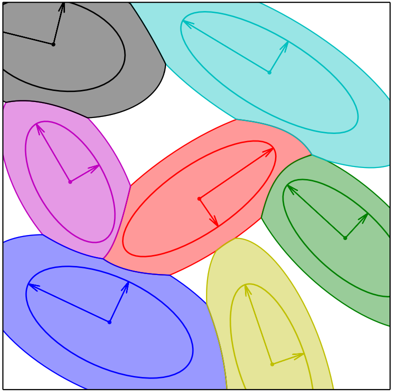

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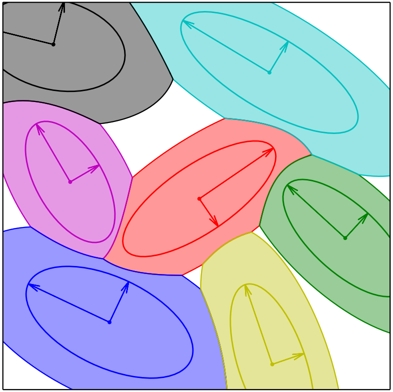

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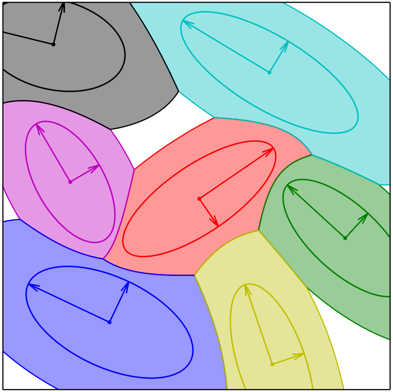

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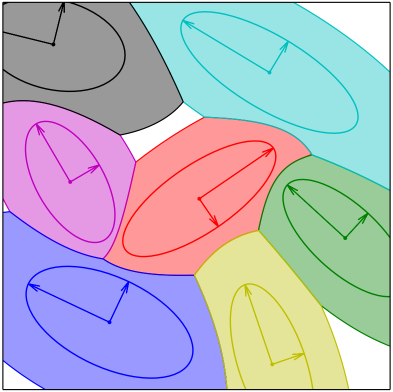

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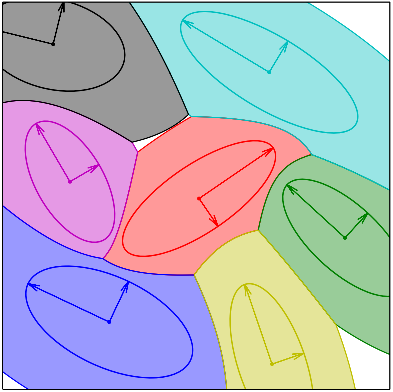

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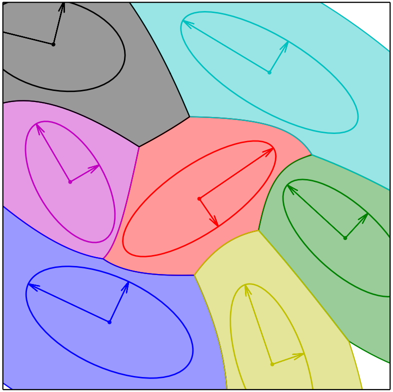

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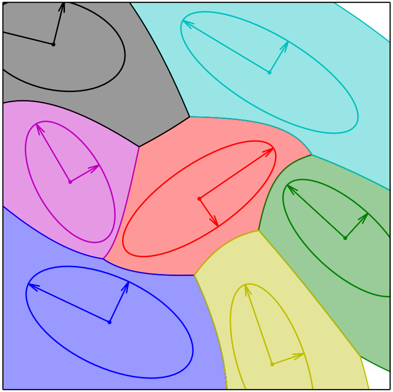

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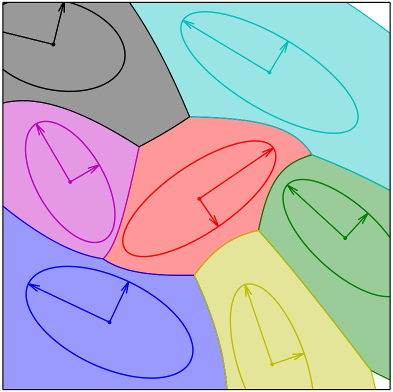

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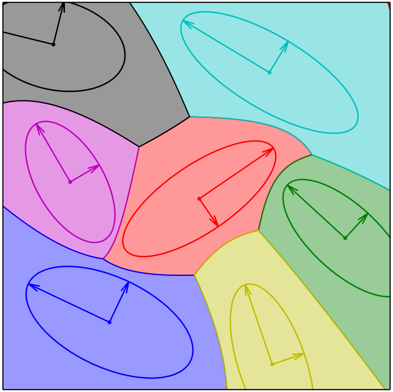

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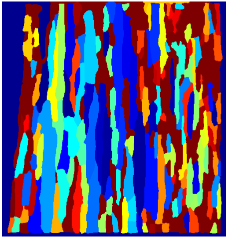
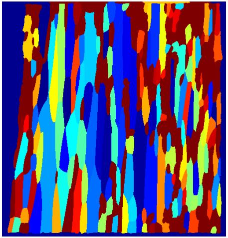
Ellipsoidal growth tessellation (EGT) — Application

Teferra and Graham-Brady (2015):

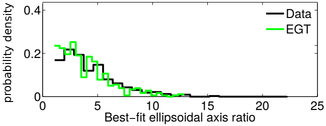
Parameterization of an hot-rolled aluminum microstructure by best-fit EGT.

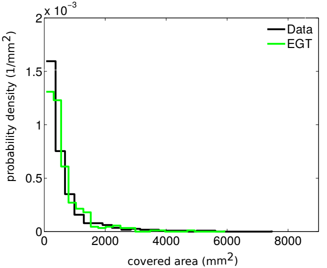


Experimental data



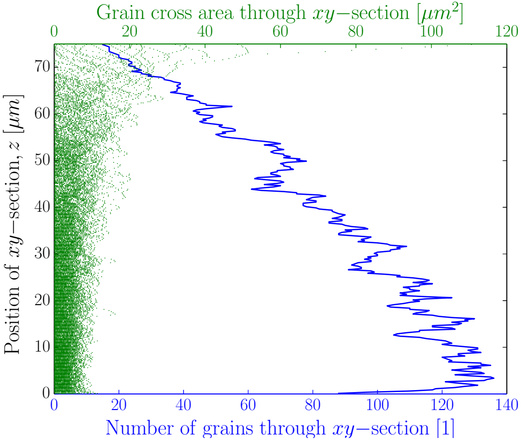
Fitted EGT

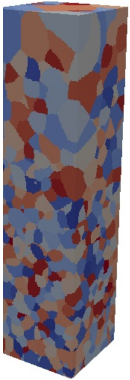




Ellipsoidal growth tessellation (EGT) — Application

Stochastic simulation of a functionally graded structure with target distributions of tessellation parameters.





Toward a semi-analytical approach — Motivation

Morphology characterization:

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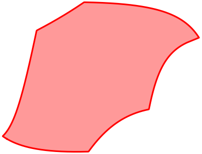

Drawback of a numerical approach:

- The accuracy of the estimated shape metrics depends on the resolution used to solve the tessellation;
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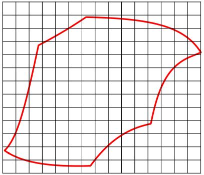

Question:

- Can we predict the morphology of an EGT model without solving it numerically for a given set of parameters $\underline{x}_\alpha$ and $\mathbf{Z}_\alpha$?

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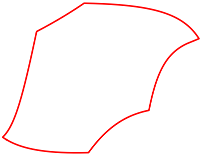

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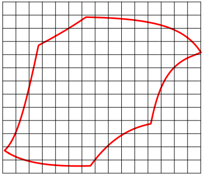

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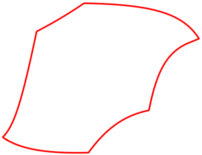

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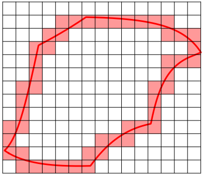

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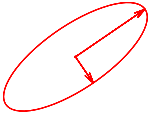
Evolving morphology of growing cells

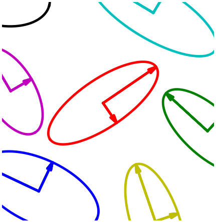
To solve for $\mathcal{I}_\alpha$, we introduce the time variable ξ at which all the points reached by the cell growing from $\underline{x}_\alpha$ lie in

$$\mathcal{D}_\alpha(\xi) = \{\underline{x} \in \mathbb{R}^d \,|\, [\underline{x} - \underline{x}_\alpha] \cdot \mathbf{Z}_\alpha \cdot [\underline{x} - \underline{x}_\alpha] = \xi^2\}$$



All the points of the evolving cell boundary $\mathcal{I}_\alpha(\xi)$ either lie in $\mathcal{D}_\alpha(\xi)$ or in common curves $\mathcal{I}_{\alpha\gamma}(\xi)$ given by:

$$\mathcal{I}_{\alpha\gamma}(\xi) = \{\underline{x} \in \mathbb{R}^d \mid T_\alpha(\underline{x}) = T_\gamma(\underline{x}) < \xi\}$$



Solving for points in $\mathcal{I}_{\alpha\gamma}$ requires to solve for a distinct quartic equation at every time ξ. Problems identifying the correct roots for large values of ξ.

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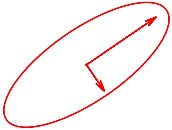

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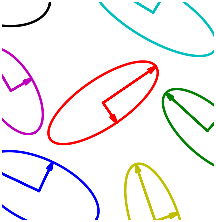

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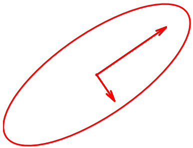

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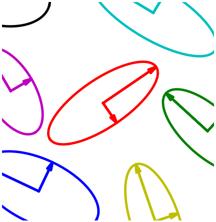
$$\mathcal{I}_{\alpha\gamma}(\xi) = \{\underline{x} \in \mathbb{R}^d \mid T_\alpha(\underline{x}) = T_\gamma(\underline{x}) < \xi\}$$

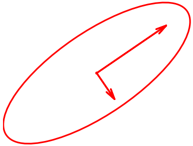


Solving for points in $\mathcal{I}_{\alpha\gamma}$ requires to solve for a distinct quartic equation at every time ξ. Problems identifying the correct roots for large values of ξ.

Evolving morphology of growing cells

To solve for $\mathcal{I}_\alpha$, we introduce the time variable ξ at which all the points reached by the cell growing from $\underline{x}_\alpha$ lie in

$$\mathcal{D}_\alpha(\xi) = \{\underline{x} \in \mathbb{R}^d \,|\, [\underline{x} - \underline{x}_\alpha] \cdot \mathbf{Z}_\alpha \cdot [\underline{x} - \underline{x}_\alpha] = \xi^2\}$$



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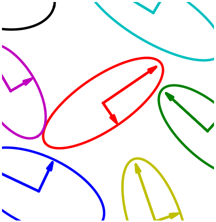

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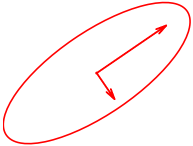

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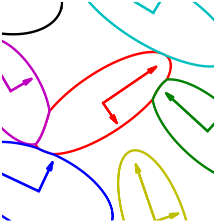

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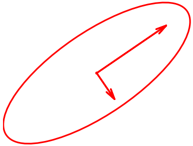

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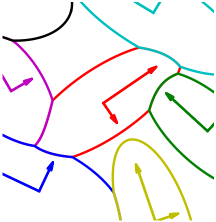

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Transformation: from growth to collision

Instead of solving directly for $\mathcal{I}_{\alpha\gamma}(\xi)$, we apply a transformation:

$$\underline{x}' = (1/\xi)\mathbf{R} \cdot \mathbf{Z}_\alpha^{1/2} \cdot (\underline{x} - \underline{x}_\alpha)$$

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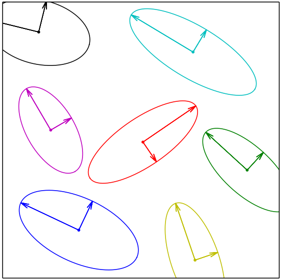

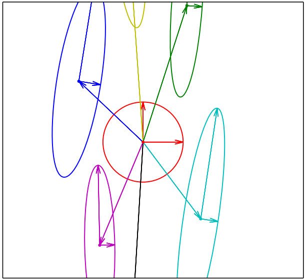

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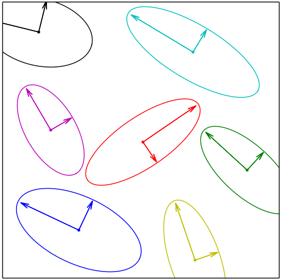

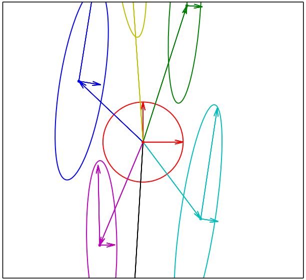

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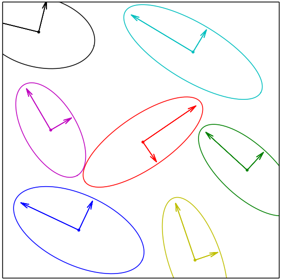

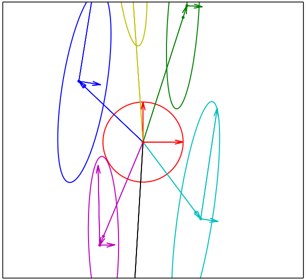

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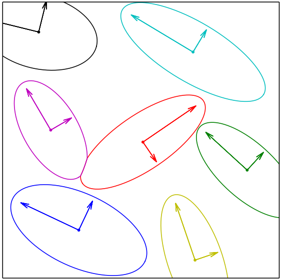

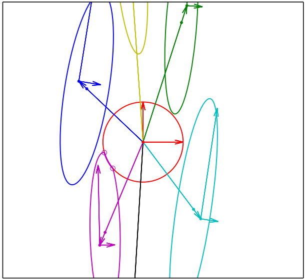

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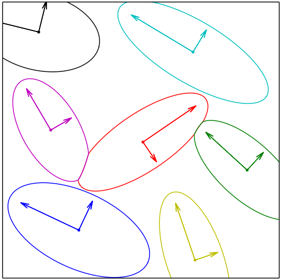

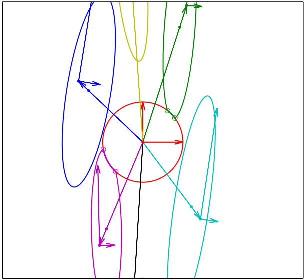

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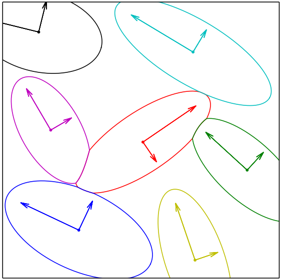

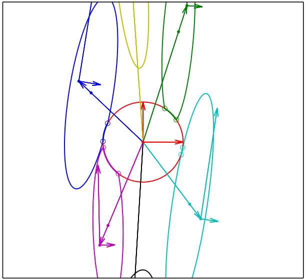

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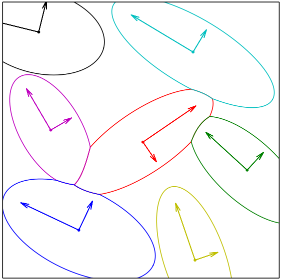

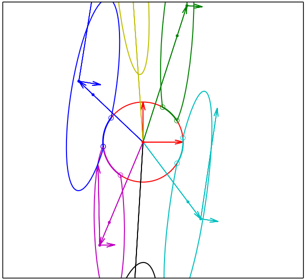

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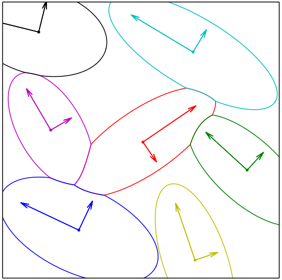

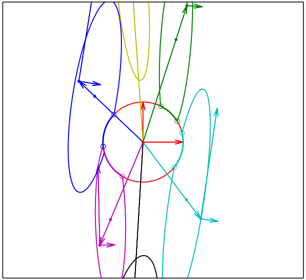

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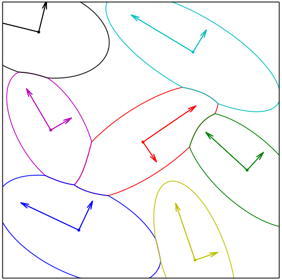

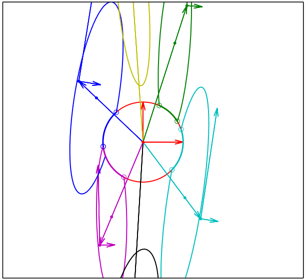

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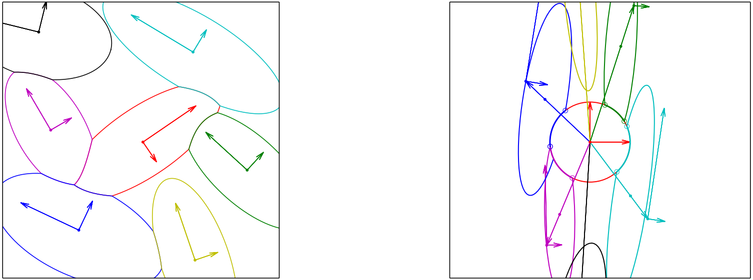

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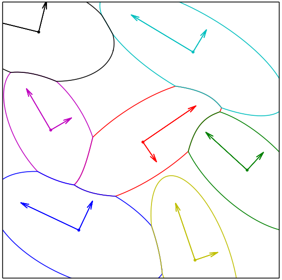

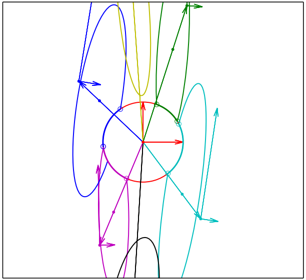

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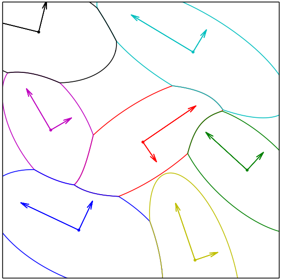
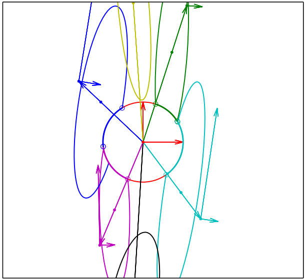
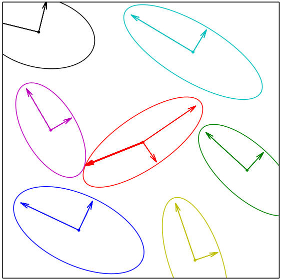
Hence $\mathcal{D}_{\gamma}(\xi)$ becomes an ellipse $\mathcal{D}'_{\gamma}(\xi)$ with fixed dimensions moving along $\mathbf{R} \cdot \mathbf{Z}_{\alpha}^{1/2} \cdot (\underline{x}_{\gamma} - \underline{x}_{\alpha})$ toward the center of the unit circle $\mathcal{D}'_{\alpha}$:

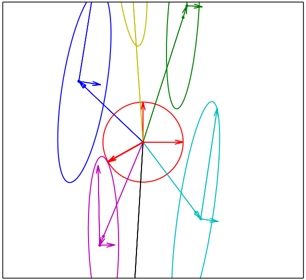




Transformation: from growth to collision

When two ellipses $\mathcal{D}_\alpha(\xi)$ and $\mathcal{D}_\gamma(\xi)$ come into contact, so does $\mathcal{D}'_\gamma(\xi)$ with the centered unit circle $\mathcal{D}'_\alpha$:





We note $\underline{x}'_{\alpha\gamma}$ the point at which $\mathcal{D}'_\gamma(\xi)$ first comes into contact with $\mathcal{D}'_\alpha$. To solve for $\underline{x}'_{\alpha\gamma}$ we find first the time at which the contact occurs:

$$\xi_{\alpha\gamma} = \min\{\xi \in \mathbb{R}^+ \mid \mathcal{D}'_\alpha \cap \mathcal{D}'_\gamma(\xi) \neq \emptyset\}$$

which is equivalent to solving for the smallest real root of a 6-th order polynomial. The contact point $\underline{x}'_{\alpha\gamma}$ is then calculated using $\xi_{\alpha\gamma}$.

Condition for ξ to be of the form $\xi(\theta')$

Every point $\underline{x}$ of the grain boundary $\mathcal{I}_\alpha$ satisfies the equation

$$\underline{x} = \underline{x}_\alpha + \xi(\underline{x}', \underline{x})\, \mathbf{Z}_\alpha^{-1/2} \cdot \mathbf{R}^T \cdot \underline{x}' \ \text{ with } \ \underline{x}' \cdot \underline{x}' = 1$$

where $\xi(\underline{x}', \underline{x})$ is the time at which contact happens at $\underline{x}'$ between $\mathcal{D}_\alpha(\xi)$ and the neighboring ellipse $\mathcal{D}_\zeta(\xi)$.

For a 2D cell $\mathcal{C}_\alpha$ *radially convex* at $\underline{x}_\alpha$, the relation $\xi(\underline{x}', \underline{x})$ simplifies to $\xi(\theta')$ where $\underline{x}' = \underline{e}_1 \cos\theta' + e_2 \sin\theta'$.

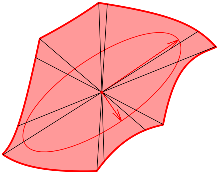
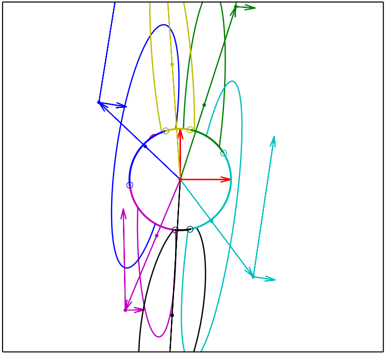


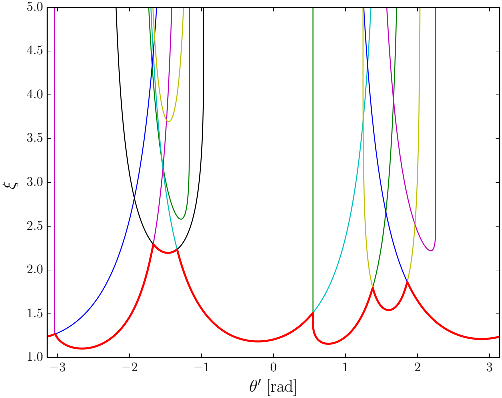
Figure : $\mathcal{C}_\alpha$ radially convex at $\underline{x}_\alpha$

The boundary $\mathcal{I}_\alpha$ of a cell *radially convex* at $\underline{x}_\alpha$ can then be reconstructed from a unit circle using the relation $\xi(\theta')$.

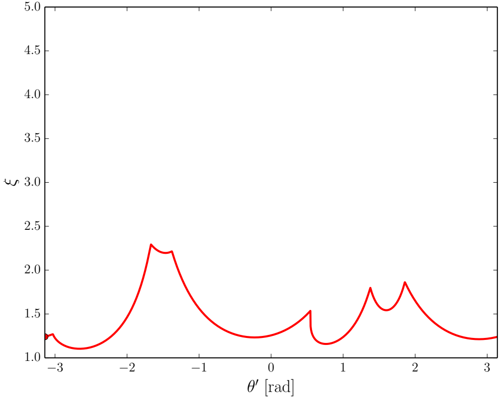
Resolution of the $\xi(\theta')$ relation

Knowing the velocity at which an ellipse $\mathcal{D}'_\gamma(\xi)$ travels through $\mathcal{D}_\alpha$, we can solve for $\xi(\theta')$ piece by piece, each part corresponding to an arc of the unit circle (or a distinct common curve of the un-tranformed boundary):

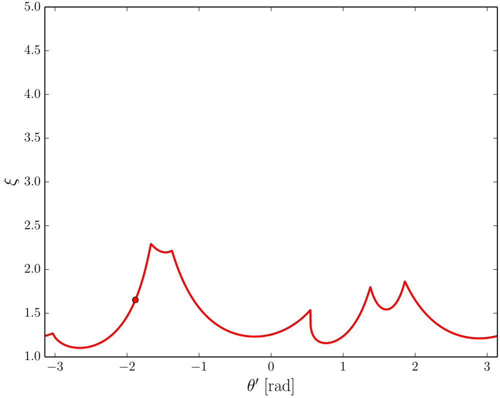




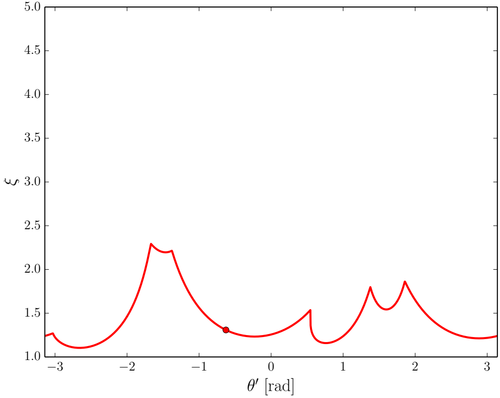
Resolution of the un-transformed grain boundary



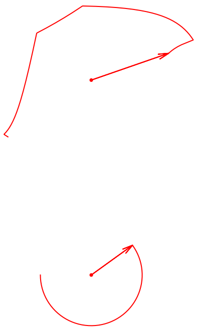
Resolution of the un-transformed grain boundary

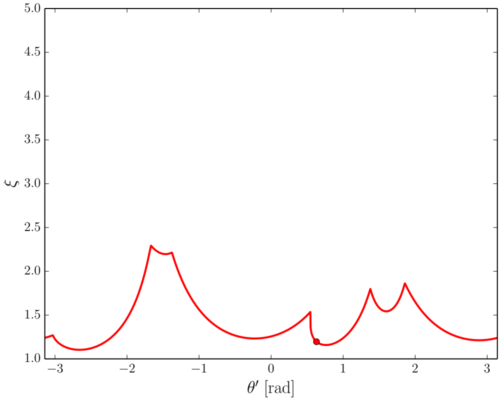


Resolution of the un-transformed grain boundary

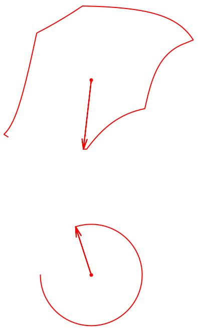


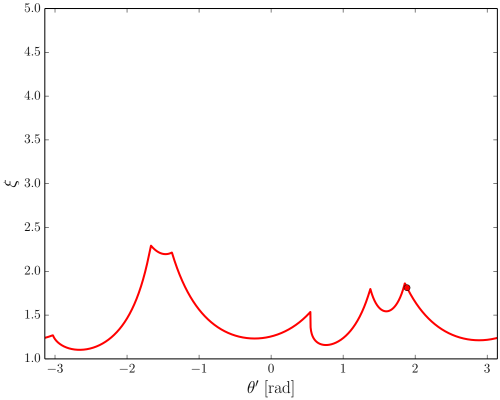
Resolution of the un-transformed grain boundary



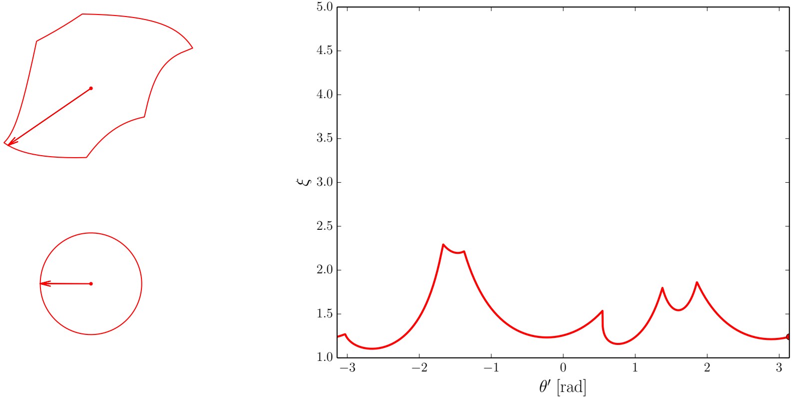


Resolution of the un-transformed grain boundary



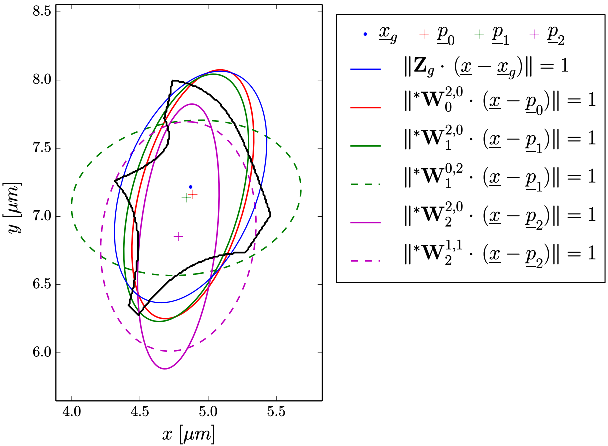


Resolution of the un-transformed grain boundary



Morphology characterization — Results

Minkowski valuations are defined as curvature integrals on the boundary of sets. They allow to quantify the different sorts of anisotropy of a grain.



Next steps and objectives

- Extend the framework to cells $\mathcal{C}_\alpha$ which are *not* radially convex at the nucleation point $\underline{x}_\alpha$;

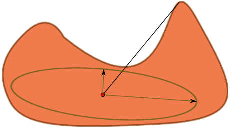


Figure : $\mathcal{C}_\alpha$ *not* radially convex at $\underline{x}_\alpha$

- Develop a simulation strategy of EGT parameters $\{(\underline{x}_\alpha, \mathbf{Z}_\alpha) \,|\, \alpha = 1, \ldots, n_\alpha\}$ for some target Minkowski valuation distributions and correlators;

- Extend the framework to three-dimensional tessellation models.

Questions/Comments