Optimal transport problems in microstructure modelling

David Bourne

Heriot-Watt University &
Maxwell Institute for Mathematical Sciences

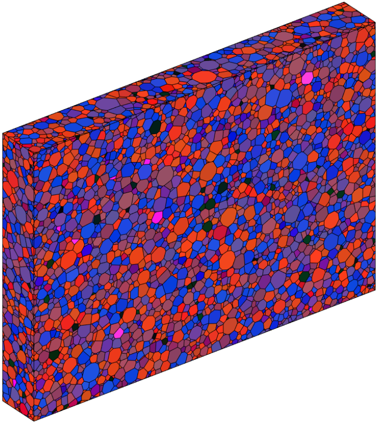
Optimal Transport Theory and Applications to Physics,
École de Physique des Houches, 13-17 March 2023

Collaborators

- Steve Roper: University of Glasgow
- Mason Pearce: PhD student, Heriot-Watt University
- Piet Kok: Tata Steel R&D (retired) & Ghent University
- Wil Spanjer: Tata Steel R&D (retired)
- Karo Sedighiani: Tata Steel R&D

Today's talk

How optimal transport theory can be used to generate geometric models of the microstructure of steels, foams, concrete, ...

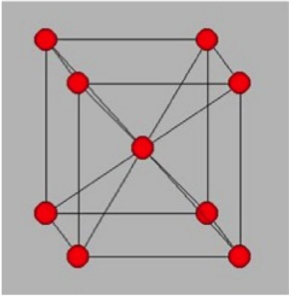


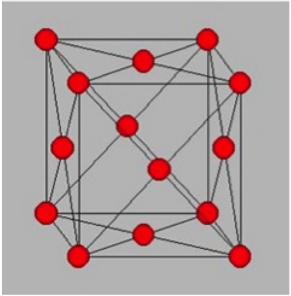
Part I: Background in steel

The microstructure of steel

The microstructure of steel

- Atoms in metals form lattices.



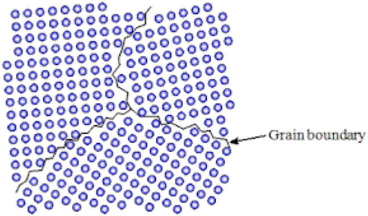


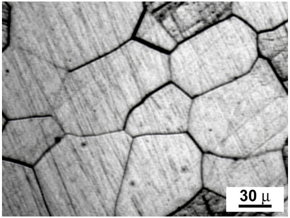
The microstructure of steel

- Atoms in metals form lattices.

The microstructure of steel

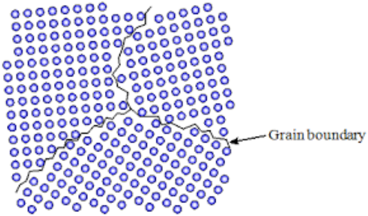
- Atoms in metals form lattices.
- Zoom out: Metals are composed of grains.

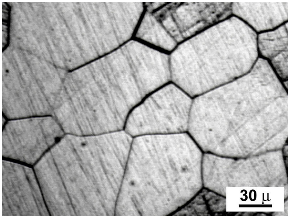




The microstructure of steel

- Atoms in metals form lattices.
- Zoom out: Metals are composed of grains.

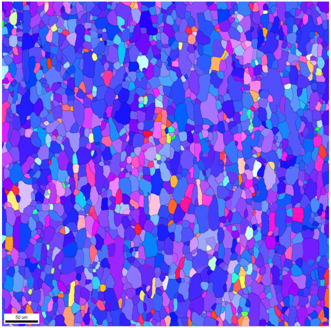




- Grains often resemble polyhedra. Under idealised cooling conditions, grains would form a Voronoi diagram.

The microstructure of steel

- High-performance steels: Grains of different sizes & shapes.



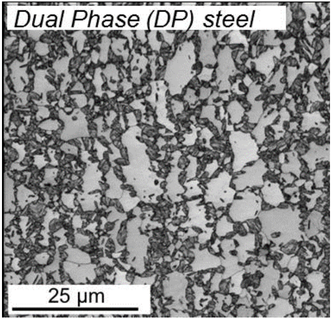
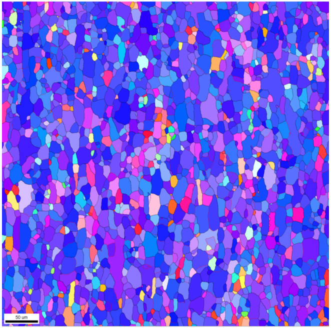


Figure: Left: DC06 steel grade. Right: Dual phase steel.

The microstructure of steel

- High-performance steels: Grains of different sizes & shapes.



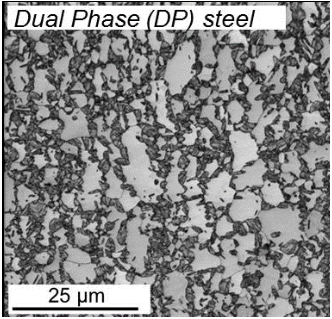
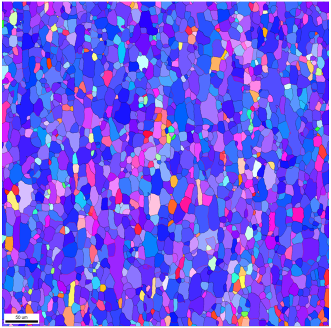


Figure: Left: DC06 steel grade. Right: Dual phase steel.

- Grain geometry affects the mechanical properties of steel.

The microstructure of steel

- High-performance steels: Grains of different sizes & shapes.



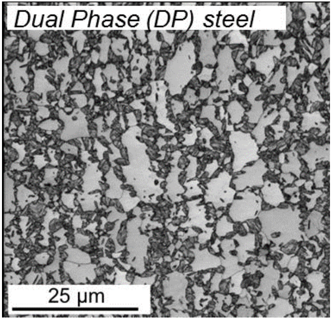


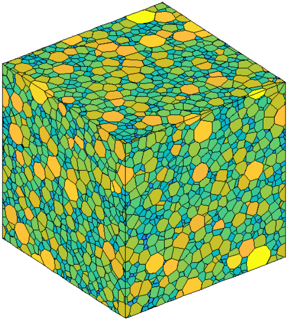
Figure: Left: DC06 steel grade. Right: Dual phase steel.

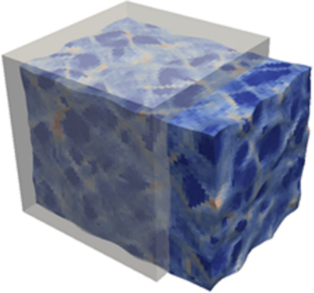
- Grain geometry affects the mechanical properties of steel.
- Goal of Tata Steel: Improve steel grades (alloys) and steel-forming processes by controlling the size and geometry of the grains.

Multiscale microstructure modelling

Approach: Computational homogenisation

- Geometric modelling: Generate a geometric model (Voronoi tessellation or Laguerre tessellation) of the steel microstructure.
- Computational plasticity: Assign mechanical propertes to each grain. Simulate standard mechanical tests (uni-axial load, shear).

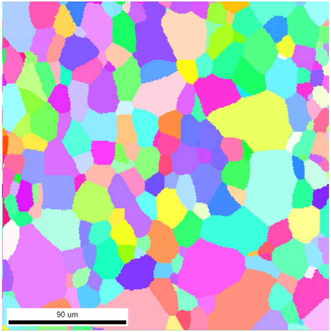




Our goal

Generate geometric models of the microstructure of polycrystalline materials (Laguerre diagrams) with prescribed geometric properties:

- grain size distributions
- spatial distributions
- aspect ratio distributions

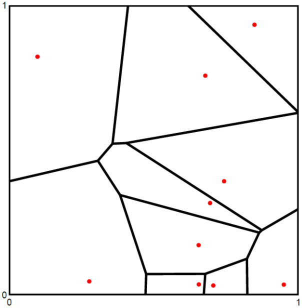


Part II: Background in semi-discrete OT

Laguerre tessellations

The Laguerre tessellation of $\Omega \subset \mathbb{R}^d$ generated by the weighted points $\{(x_i, w_i)\}_{i=1}^n$, $x_i \in \Omega$, $w_i \in \mathbb{R}$, is the partition $\{L_i\}_{i=1}^n$ of Ω defined by

$$L_i = \{x \in \Omega : |x - x_i|^2 - w_i \leq |x - x_j|^2 - w_j \ \forall j\}.$$



Laguerre cells are convex polygons in 2D and polyhedra in 3D.

Semi-discrete optimal transport

Semi-discrete optimal transport

- Source measure: Lebesgue measure $\mathcal{L}^d \llcorner \Omega, \ \Omega \subset \mathbb{R}^d$

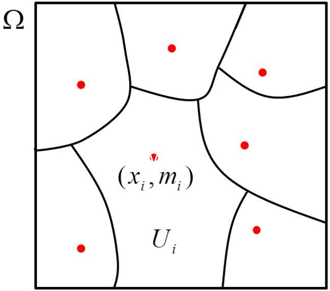
Semi-discrete optimal transport

- Source measure: Lebesgue measure $\mathcal{L}^d \llcorner \Omega,\ \ \Omega \subset \mathbb{R}^d$
- Discrete target measure: $\sum_{i=1}^n v_i \delta_{x_i},\ \ x_i \in \Omega,\ \ \sum_i v_i = \mathcal{L}^d(\Omega)$

Semi-discrete optimal transport

- Source measure: Lebesgue measure $\mathcal{L}^d \llcorner \Omega, \; \Omega \subset \mathbb{R}^d$
- Discrete target measure: $\sum_{i=1}^n v_i \delta_{x_i}, \; x_i \in \Omega, \; \sum_i v_i = \mathcal{L}^d(\Omega)$
- Semi-discrete transport problem:

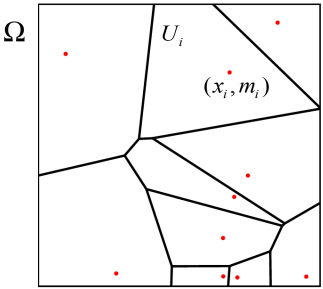
$$W_2^2\left(\mathcal{L}^d \llcorner \Omega, \sum_i v_i \delta_{x_i}\right) = \min_{\substack{\text{partitions } \{U_i\} \text{ of } \Omega \\ \mathcal{L}^d(U_i) = v_i \; \forall \, i}} \sum_i \int_{U_i} |x - x_i|^2 \, dx$$



Semi-discrete optimal transport

- Source measure: Lebesgue measure $\mathcal{L}^d \llcorner \Omega,\ \ \Omega \subset \mathbb{R}^d$
- Discrete target measure: $\sum_{i=1}^n v_i \delta_{x_i},\ \ x_i \in \Omega,\ \ \sum_i v_i = \mathcal{L}^d(\Omega)$
- Semi-discrete transport problem:

$$W_2^2\left(\mathcal{L}^d \llcorner \Omega, \sum_i v_i \delta_{x_i}\right) = \min_{\substack{\text{partitions } \{U_i\} \text{ of } \Omega \\ \mathcal{L}^d(U_i)=v_i\ \forall\ i}} \sum_i \int_{U_i} |x - x_i|^2\, dx$$



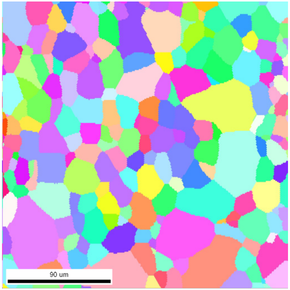
The optimal partition is a Laguerre tessellation $\{L_i\}$ with cells of volume $\{v_i\}$

Part III: Main results

Our goal

Generate geometric models of the microstructure of polycrystalline materials (Laguerre diagrams) with prescribed geometric properties:

- grain size distributions
- spatial distributions
- aspect ratio distributions



Bourne, Kok, Roper & Spanjer (2020), Bourne, Pearce & Roper (2023)

Controlling the grain size distribution

Question posed to us by Tata Steel: How do you generate a Laguerre diagram with polyhedra (grains) of given volumes $v_1, \ldots, v_n$?

Controlling the grain size distribution

Question posed to us by Tata Steel: How do you generate a Laguerre diagram with polyhedra (grains) of given volumes $v_1, \ldots, v_n$?

Solution: Semi-discrete optimal transport

Controlling the grain size distribution

Question posed to us by Tata Steel: How do you generate a Laguerre diagram with polyhedra (grains) of given volumes $v_1, \ldots, v_n$?

Solution: Semi-discrete optimal transport

- For *any* $x_1, \ldots, x_n$, solve the semi-discrete transport problem

$$W_2\Big(1, \sum_{i=1}^{n} v_i \delta_{x_i}\Big).$$

If $\{L_i\}_{i=1}^n$ is the optimal Laguerre tessellation, then $\mathcal{L}^d(L_i) = v_i$.

Controlling the grain size distribution

Question posed to us by Tata Steel: How do you generate a Laguerre diagram with polyhedra (grains) of given volumes $v_1, \ldots, v_n$?

Solution: Semi-discrete optimal transport

- For *any* $x_1, \ldots, x_n$, solve the semi-discrete transport problem

$$W_2\Big(1, \sum_{i=1}^{n} v_i \delta_{x_i}\Big).$$

  If $\{L_i\}_{i=1}^n$ is the optimal Laguerre tessellation, then $\mathcal{L}^d(L_i) = v_i$.

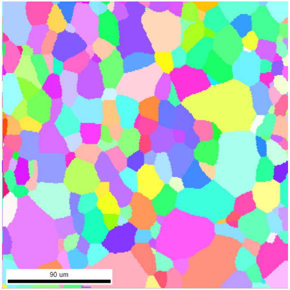
- Very fast algorithms (damped Newton method) and software:

  Kitagawa, Mérigot & Thibert (2019), A. Gallouët, Mérigot & Thibert (2022), Lévy, Mohayaee & von Hausegger (2021), Lévy (2015), Mérigot (2011), ...
  pysdot (Mérigot & Leclerc), Geogram (Lévy), sdot (Meyron), MATLAB-SDOT

Our goal

Generate geometric models of the microstructure of polycrystalline materials (Laguerre diagrams) with prescribed geometric properties:

- grain size distributions
- spatial distributions
- aspect ratio distributions



Bourne, Kok, Roper & Spanjer (2020), Bourne, Pearce & Roper (2023)

Controlling the grain size and spatial distribution

Question posed to us by Tata Steel: How do you generate a Laguerre diagram with polyhedra (grains) of given volumes $v_1, \ldots, v_n$?

Solution: Semi-discrete optimal transport.

- For *any* $x_1, \ldots, x_n$, solve the semi-discrete transport problem

$$W_2\Big(1, \sum_{i=1}^{n} v_i \delta_{x_i}\Big).$$

If $\{L_i\}_{i=1}^{n}$ is the optimal Laguerre tessellation, then $\mathcal{L}^d(L_i) = v_i$.

Controlling the grain size and spatial distribution

Question posed to us by Tata Steel: How do you generate a Laguerre diagram with polyhedra (grains) of given volumes $v_1, \dots, v_n$?

Solution: Semi-discrete optimal transport.

- For *any* $x_1, \dots, x_n$, solve the semi-discrete transport problem

$$W_2\left(1, \sum_{i=1}^{n} v_i \delta_{x_i}\right).$$

  If $\{L_i\}_{i=1}^n$ is the optimal Laguerre tessellation, then $\mathcal{L}^d(L_i) = v_i$.

- Choice of $x_1, \dots, x_n$ gives some control over the spatial distribution.

Controlling the grain size and spatial distribution

Question posed to us by Tata Steel: How do you generate a Laguerre diagram with polyhedra (grains) of given volumes $v_1, \dots, v_n$?

Solution: Semi-discrete optimal transport.

- For *any* $x_1, \dots, x_n$, solve the semi-discrete transport problem

$$W_2\left(1, \sum_{i=1}^{n} v_i \delta_{x_i}\right).$$

  If $\{L_i\}_{i=1}^n$ is the optimal Laguerre tessellation, then $\mathcal{L}^d(L_i) = v_i$.

- Choice of $x_1, \dots, x_n$ gives some control over the spatial distribution.
- Generate 'regular' microstructures by solving a quantization problem:

$$\min_{\{x_1,\dots,x_n\}} W_2\left(1, \sum_{i=1}^{n} v_i \delta_{x_i}\right)$$

Controlling the grain size and spatial distribution

Question posed to us by Tata Steel: How do you generate a Laguerre diagram with polyhedra (grains) of given volumes $v_1, \ldots, v_n$?

Solution: Semi-discrete optimal transport.

- For *any* $x_1, \ldots, x_n$, solve the semi-discrete transport problem

$$W_2\left(1, \sum_{i=1}^{n} v_i \delta_{x_i}\right).$$

If $\{L_i\}_{i=1}^n$ is the optimal Laguerre tessellation, then $\mathcal{L}^d(L_i) = v_i$.

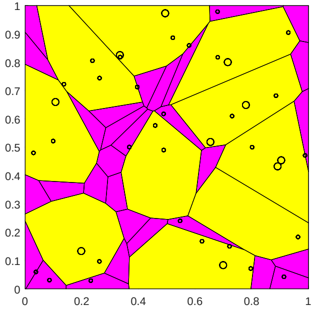
- Choice of $x_1, \ldots, x_n$ gives some control over the spatial distribution.
- Generate 'regular' microstructures by solving a quantization problem:

$$\min_{\{x_1,\ldots,x_n\}} W_2\left(1, \sum_{i=1}^{n} v_i \delta_{x_i}\right)$$

Algorithms/convergence: Mérigot, Santambrogio & Sarrazin (2021), B., Kok, Roper & Spanjer (2020), Xin, Lévy et al. (2016), Mérigot & Mirebeau (2016)

Example

Dual phase microstructure: 30 grains area a, 10 grains area $10a$



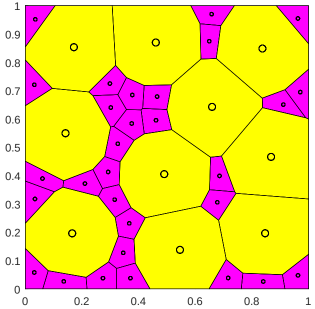


Figure: Left: x_i drawn at random. Right: Locally-optimal quantizer.

Quantization problem

$$\min_{\{x_1,\dots,x_n\}} E(x_1,\dots,x_n), \qquad E(x_1,\dots,x_n) = W_2\Big(1, \sum_{i=1}^{n} v_i \delta_{x_i}\Big)$$

Quantization problem

$$\min_{\{x_1,\ldots,x_n\}} E(x_1,\ldots,x_n), \qquad E(x_1,\ldots,x_n) = W_2\Big(1, \sum_{i=1}^{n} v_i \delta_{x_i}\Big)$$

- Critical points of E: Centroidal Laguerre tessellations

Quantization problem

$$\min_{\{x_1,\ldots,x_n\}} E(x_1,\ldots,x_n), \qquad E(x_1,\ldots,x_n) = W_2\left(1, \sum_{i=1}^n v_i \delta_{x_i}\right)$$

- Critical points of E: Centroidal Laguerre tessellations
- Generalised Lloyd's algorithm. Iteration k:
  - $\{L_i^{(k)}\}$ = optimal partition for OT problem $W_2\left(1, \sum_{i=1}^n v_i \delta_{x_i^{(k)}}\right)$
  - $x_i^{(k+1)}$ = centroid$(L_i^{(k)}) \ \forall\, i$

Quantization problem

$$\min_{\{x_1,\ldots,x_n\}} E(x_1,\ldots,x_n), \qquad E(x_1,\ldots,x_n) = W_2\left(1, \sum_{i=1}^{n} v_i \delta_{x_i}\right)$$

- Critical points of E: Centroidal Laguerre tessellations
- Generalised Lloyd's algorithm. Iteration k:
  - $\{L_i^{(k)}\}$ = optimal partition for OT problem $W_2\left(1, \sum_{i=1}^{n} v_i \delta_{x_i^{(k)}}\right)$
  - $x_i^{(k+1)}$ = centroid$(L_i^{(k)})\ \ \forall\, i$
- Convergence: Mérigot, Santambrogio & Sarrazin (2021), Bourne, Kok, Roper & Spanjer (2020)

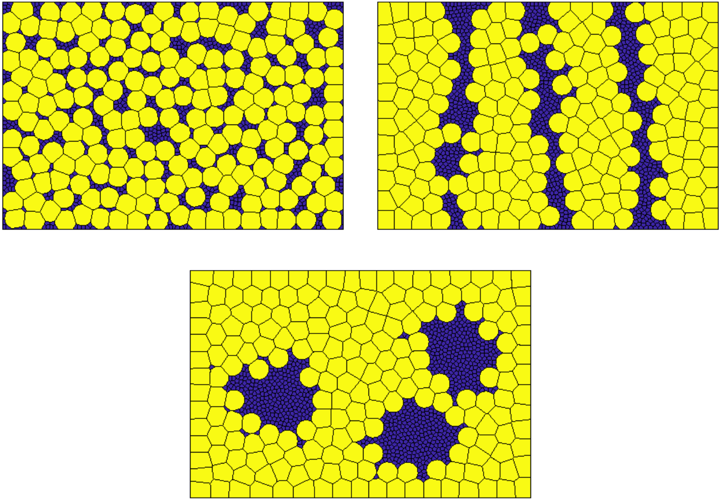
Quantization problem

$$\min_{\{x_1,\dots,x_n\}} E(x_1,\dots,x_n), \qquad E(x_1,\dots,x_n) = W_2\left(1, \sum_{i=1}^n v_i \delta_{x_i}\right)$$

- Critical points of E: Centroidal Laguerre tessellations
- Generalised Lloyd's algorithm. Iteration k:
  - $\{L_i^{(k)}\}$ = optimal partition for OT problem $W_2\left(1, \sum_{i=1}^n v_i \delta_{x_i^{(k)}}\right)$
  - $x_i^{(k+1)}$ = centroid$(L_i^{(k)})$ $\forall\, i$
- Convergence: Mérigot, Santambrogio & Sarrazin (2021), Bourne, Kok, Roper & Spanjer (2020)
- Non-convexity: Non-convexity is our friend!

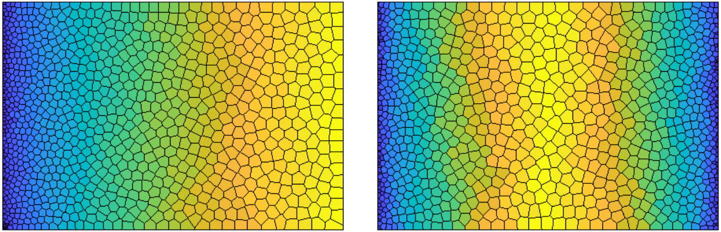
Using non-convexity to control spatial distribution

Initial choice of seeds $x_i^{(0)}$ has a big effect on the pattern:



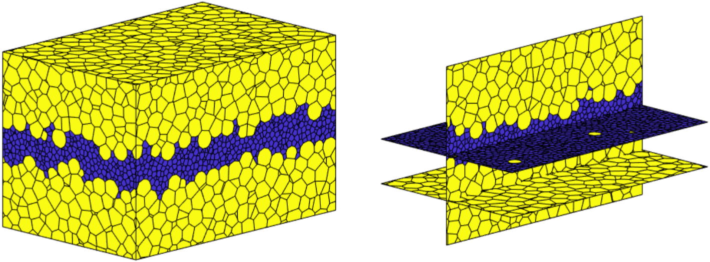
Using non-convexity to control spatial distribution

Initial choice of seeds $x_i^{(0)}$ has a big effect on the pattern:



Using non-convexity to control spatial distribution

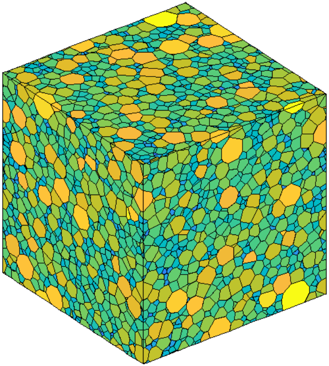
Initial choice of seeds $x_i^{(0)}$ has a big effect on the pattern:



Optimal transport with periodic quadratic cost

Same method works for periodic Laguerre tessellations (important for computational homogenisation), where

$$L_i^{\mathrm{per}} = \{x \in \Omega \,:\, |x - x_i|_{\mathrm{per}}^2 - w_i \leq |x - x_j|_{\mathrm{per}}^2 - w_j \;\forall\, j\}.$$

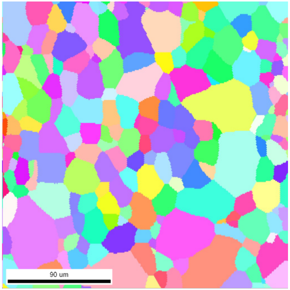


Bourne, Pearce & Roper (2023)

Our goal

Generate geometric models of the microstructure of polycrystalline materials (Laguerre diagrams) with prescribed geometric properties:

- grain size distributions
- spatial distributions
- aspect ratio distributions



Fitting volumes and centroids

Question: Given a list of target volumes $v_1, \ldots, v_n$ and target centroids $c_1, \ldots, c_n$, find a Laguerre tessellation $\{L_i\}_{i=1}^n$ with grains of correct volume and 'minimum centroid error'.

Fitting volumes and centroids

Question: Given a list of target volumes $v_1, \dots, v_n$ and target centroids $c_1, \dots, c_n$, find a Laguerre tessellation $\{L_i\}_{i=1}^n$ with grains of correct volume and 'minimum centroid error'.

Notation: The centroid (barycentre) of a grain L_i is

$$b(L_i) = \frac{1}{\mathcal{L}^d(L_i)} \int_{L_i} x \,\mathrm{d}x.$$

Preliminary results: Special case

Theorem (B., Pearce, Roper)

Given a list of target volumes $v_1, \ldots, v_n$ and target centroids $c_1, \ldots, c_n$, suppose there exists a Laguerre tessellation $\{L_i(X^*, w^*)\}_{i=1}^{n}$ such that $\mathcal{L}^d(L_i) = v_i$ and $b(L_i) = c_i$ for all i. Then

Preliminary results: Special case

Theorem (B., Pearce, Roper)

Given a list of target volumes $v_1, \ldots, v_n$ and target centroids $c_1, \ldots, c_n$, suppose there exists a Laguerre tessellation $\{L_i(X^*, w^*)\}_{i=1}^n$ such that $\mathcal{L}^d(L_i) = v_i$ and $b(L_i) = c_i$ for all i. Then

1. The Laguerre diagram is unique.

Preliminary results: Special case

Theorem (B., Pearce, Roper)

Given a list of target volumes $v_1, \ldots, v_n$ and target centroids $c_1, \ldots, c_n$, suppose there exists a Laguerre tessellation $\{L_i(X^*, w^*)\}_{i=1}^n$ such that $\mathcal{L}^d(L_i) = v_i$ and $b(L_i) = c_i$ for all i. Then

1. The Laguerre diagram is unique.

   (The *grains* are unique. The seeds can be uniformly translated and dilated, $x_i' = \lambda x_i + t$ for all i, without changing the grains L_i.)

Preliminary results: Special case

Theorem (B., Pearce, Roper)

Given a list of target volumes $v_1, \ldots, v_n$ and target centroids $c_1, \ldots, c_n$, suppose there exists a Laguerre tessellation $\{L_i(X^*, w^*)\}_{i=1}^n$ such that $\mathcal{L}^d(L_i) = v_i$ and $b(L_i) = c_i$ for all i. Then

1. The Laguerre diagram is unique.

Preliminary results: Special case

Theorem (B., Pearce, Roper)

Given a list of target volumes $v_1, \ldots, v_n$ and target centroids $c_1, \ldots, c_n$, suppose there exists a Laguerre tessellation $\{L_i(X^*, w^*)\}_{i=1}^n$ such that $\mathcal{L}^d(L_i) = v_i$ and $b(L_i) = c_i$ for all i. Then

1. The Laguerre diagram is unique.
2. The seeds $X^* = (x_1^*, \ldots, x_n^*)$ maximise the concave function $H : (\mathbb{R}^d)^n \to \mathbb{R}$,

$$H(X) = \frac{1}{2} W_2^2 \Big(1, \sum_{i=1}^n v_i \delta_{x_i} \Big) + \sum_{i=1}^n v_i c_i \cdot x_i - \frac{1}{2} \sum_{i=1}^n v_i |x_i|^2.$$

Preliminary results: Special case

Theorem (B., Pearce, Roper)

Given a list of target volumes $v_1, \dots, v_n$ and target centroids $c_1, \dots, c_n$, suppose there exists a Laguerre tessellation $\{L_i(X^*, w^*)\}_{i=1}^n$ such that $\mathcal{L}^d(L_i) = v_i$ and $b(L_i) = c_i$ for all i. Then

1. The Laguerre diagram is unique.
2. The seeds $X^* = (x_1^*, \dots, x_n^*)$ maximise the concave function $H : (\mathbb{R}^d)^n \to \mathbb{R}$,

$$H(X) = \frac{1}{2} W_2^2\Big(1, \sum_{i=1}^n v_i \delta_{x_i}\Big) + \sum_{i=1}^n v_i c_i \cdot x_i - \frac{1}{2} \sum_{i=1}^n v_i |x_i|^2.$$

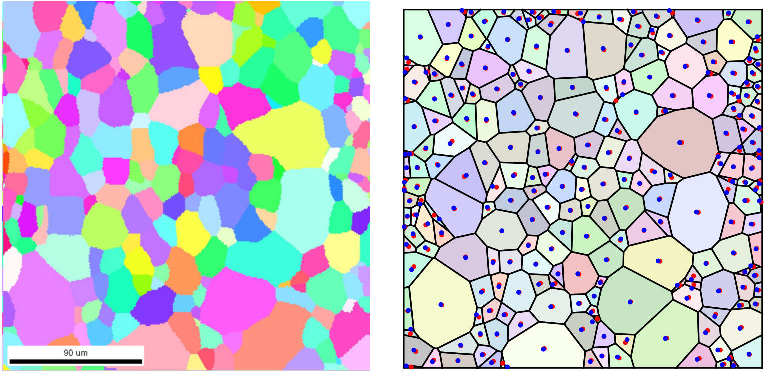
H is C^1 on the set $\{(x_1, \dots, x_n) \in (\mathbb{R}^d)^n : x_i \neq x_j \; \forall\, i \neq j\}$ and

$$\frac{\partial H}{\partial x_i} = v_i(c_i - b(L_i)).$$

(Mérigot, Santambrogio & Sarrazin (2021))

Preliminary results: General case

Given a list of target volumes $v_1, \ldots, v_n$ and target centroids $c_1, \ldots, c_n$, find a Laguerre tessellation $\{L_i\}_{i=1}^n$ such that $\mathcal{L}^d(L_i) = v_i$ for all i and $\sum_i |v_i(b(L_i) - c_i)|^2$ is minimal.

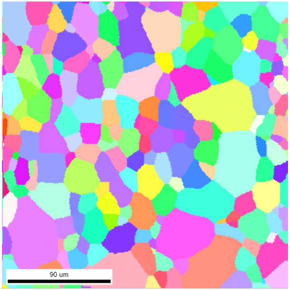


Left: EBSD image. Right: Fitted diagram. The blue dots are the target centroids, the red dots are the actual centroids.

Our goal

Generate geometric models of the microstructure of polycrystalline materials (Laguerre diagrams) with prescribed geometric properties:

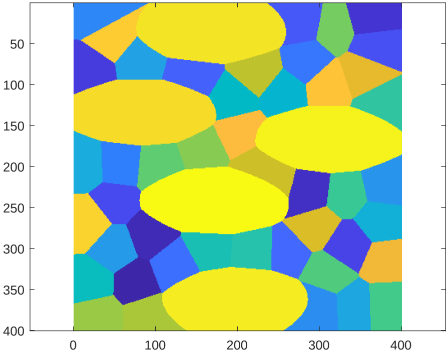
- grain size distributions
- spatial distributions
- aspect ratio distributions



Controlling the grain size and aspect ratio distribution

Controlling the grain size and aspect ratio distribution

We can represent anisotropic microstructures by anisotropic Laguerre diagrams.



A. Alpers, A. Brieden, P. Gritzmann, A. Lyckegaard, and H.F. Poulsen. Generalized balanced power diagrams for 3D representations of polycrystals. *Philos. Mag.* 95(9): 1016-1028, 2015.

Controlling the grain size and aspect ratio distribution

The anisotropic Laguerre tessellation generated by the weighted points $\{(x_i, w_i, A_i)\}_{i=1}^n$, where $x_i \in \Omega$, $w_i \in \mathbb{R}$, A_i are SPD matrices, is the partition $\{L_i\}_{i=1}^n$ of Ω defined by

$$L_i = \left\{ x \in \Omega : |x - x_i|_{A_i}^2 - w_i \le |x - x_j|_{A_j}^2 - w_j \;\forall\, j \right\}$$

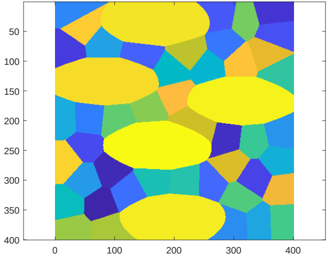
where $|\cdot|_A$ is the A-norm: $|x - x_i|_A^2 = (x - x_i) \cdot A(x - x_i)$.

Controlling the grain size and aspect ratio distribution

The anisotropic Laguerre tessellation generated by the weighted points $\{(x_i, w_i, A_i)\}_{i=1}^n$, where $x_i \in \Omega$, $w_i \in \mathbb{R}$, A_i are SPD matrices, is the partition $\{L_i\}_{i=1}^n$ of Ω defined by

$$L_i = \left\{ x \in \Omega : |x - x_i|_{A_i}^2 - w_i \leq |x - x_j|_{A_j}^2 - w_j \;\forall\, j \right\}$$

where $|\cdot|_A$ is the A-norm: $|x - x_i|_A^2 = (x - x_i) \cdot A(x - x_i)$.



The A_i matrices give some control over the aspect ratio of the cells.

Controlling the grain size for anisotropic diagrams

Q. Can we choose the generators $(x_1, w_1, A_1), \ldots, (x_n, w_n, A_n)$ so that the anisotropic Laguerre cells have desired volumes $v_1, \ldots, v_n$?

Controlling the grain size for anisotropic diagrams

Q. Can we choose the generators $(x_1, w_1, A_1), \ldots, (x_n, w_n, A_n)$ so that the anisotropic Laguerre cells have desired volumes $v_1, \ldots, v_n$?

A. Yes. Solution(s) using optimal transport theory:

Controlling the grain size for anisotropic diagrams

Q. Can we choose the generators $(x_1, w_1, A_1), \ldots, (x_n, w_n, A_n)$ so that the anisotropic Laguerre cells have desired volumes $v_1, \ldots, v_n$?

A. Yes. Solution(s) using optimal transport theory:

- For *any* $\{x_i\}$, $\{A_i\}$, solve the semi-discrete transport problem

$$W_c\Big(1, \sum_{i=1}^{n} v_i \delta_{x_i}\Big)$$

  with anisotropic cost $c(x, x_i) = |x - x_i|^2_{A_i}$.

Controlling the grain size for anisotropic diagrams

Q. Can we choose the generators $(x_1, w_1, A_1), \dots, (x_n, w_n, A_n)$ so that the anisotropic Laguerre cells have desired volumes $v_1, \dots, v_n$?

A. Yes. Solution(s) using optimal transport theory:

- For *any* $\{x_i\}$, $\{A_i\}$, solve the semi-discrete transport problem

$$W_c\Big(1, \sum_{i=1}^{n} v_i \delta_{x_i}\Big)$$

  with anisotropic cost $c(x, x_i) = |x - x_i|^2_{A_i}$.

- The optimal partition $\{L_i\}_{i=1}^{n}$ is an anisotropic Laguerre tessellation and $\mathcal{L}^d(L_i) = v_i \; \forall \, i$.

Controlling the grain size for anisotropic diagrams

Q. Can we choose the generators $(x_1, w_1, A_1), \dots, (x_n, w_n, A_n)$ so that the anisotropic Laguerre cells have desired volumes $v_1, \dots, v_n$?

A. Yes. Solution(s) using optimal transport theory:

- For *any* $\{x_i\}$, $\{A_i\}$, solve the semi-discrete transport problem

$$W_c\Big(1, \sum_{i=1}^{n} v_i \delta_{x_i}\Big)$$

  with anisotropic cost $c(x, x_i) = |x - x_i|^2_{A_i}$.

- The optimal partition $\{L_i\}_{i=1}^n$ is an anisotropic Laguerre tessellation and $\mathcal{L}^d(L_i) = v_i \ \forall \ i$.

- Implementation: Maximise the concave function $\mathcal{K} : \mathbb{R}^n \to \mathbb{R}$,

$$\mathcal{K}(w) = \sum_{i=1}^{n} \int_{L_i(w)} \left(|x - x_i|^2_{A_i} - w_i\right) \mathrm{d}x + \sum_{i=1}^{n} v_i w_i$$

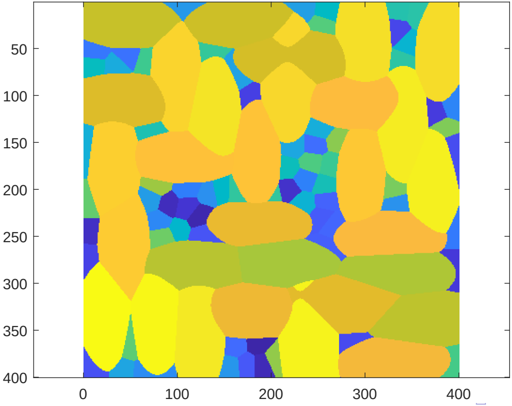
  where

$$L_i(w) = \{x \in \Omega \, : \, |x - x_i|^2_{A_i} - w_i \le |x - x_j|^2_{A_j} - w_j \ \forall \, j\}.$$

Example

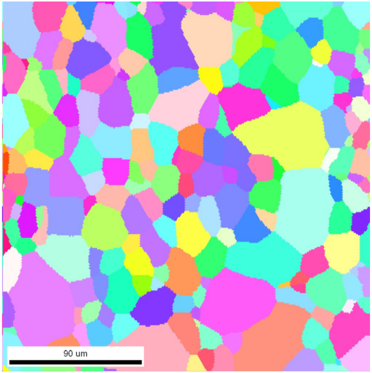
Dual phase microstructure: 100 cells: 70 small cells of area a, 30 large cells of area $10a$ (error less than 1%). The large cells have two different A_i (15 of each type):

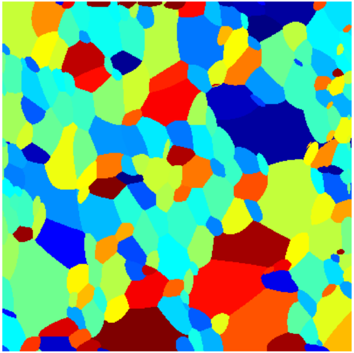
$$A_{\text{small}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad A_{\text{large},1} = \begin{bmatrix} 5 & 0 \\ 0 & 1 \end{bmatrix}, \quad A_{\text{large},2} = \begin{bmatrix} 1 & 0 \\ 0 & 5 \end{bmatrix}$$



Fitting anisotropic diagrams to EBSD data

Basic fitting: Take x_i, A_i, v_i from EBSD data (grain centroids, ellipsoids, volumes) - solve the semi-discrete OT problem for w_i.





Left: EBSD image from Tata Steel. Right: Anisotropic Laguerre.

Implementation issues

Question: How can we compute anisotropic diagrams efficiently?

Implementation issues

Question: How can we compute anisotropic diagrams efficiently?

- Pixel method. Compute the "anisotropic distance" $(p_i - x_j) \cdot A_j(p_i - x_j) - w_j$ between every pixel i and seed j.
- Geometric lifting method. Compute a standard power diagram in dimension $d + d(d+1)/2$, intersect with a surface, project. Boissonnat, Wormser & Yvinec (2007)
- Entropic semi-discrete optimal transport.
- Stochastic optimisation. Genevay, Cuturi, Peyré & Bach (2016)
- Boundary method. Dieci & Walsh III (2019)
- ...