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# Statistical interpretation of microstructures

## A mathematical model for estimating grain size distributions

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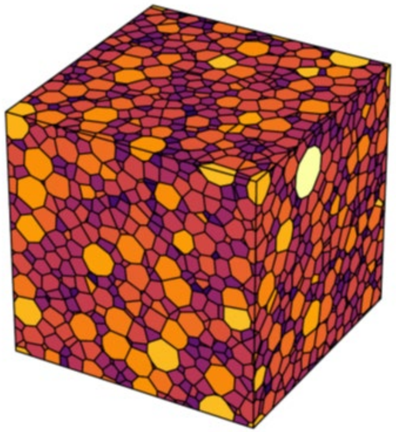
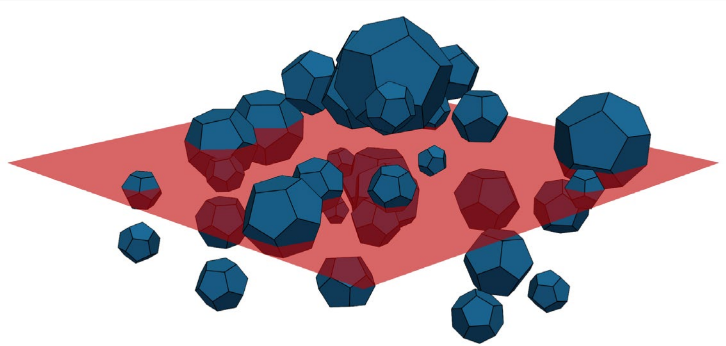
# Introduction

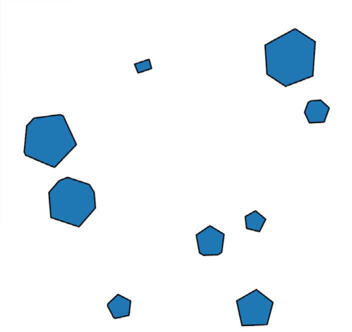
- Given microscopic image data, e.g. 2D EBSD data we would like to get information of a 3D microstructure.
- Various quantities may be of interest. We are interested in estimating the volume distribution of the 3D grains given the observed 2D grains in a section.
- Such a method may assist in generating a 'digital twin' of the microstructure.



# Introduction

- **Model:** All particles have the same convex shape, but a different size. The challenge: 2D → 3D
- **Problem:** How to estimate the volume distribution of these 3D particles using the areas of the observed 2D section profiles?
- **Why?:** Resolving this serves as a stepping stone towards handling more realistic models for materials microstructures.





# Mathematical problem description

- Choose a reference convex particle, scaled to have volume 1.
- The following equation describes the problem:

$$f_A(s) = \frac{1}{\mathbb{E}(\Lambda)} \int_{\sqrt{\frac{s}{a_{\max}}}}^{\infty} g\left(\frac{s}{\lambda^2}\right) \frac{h(\lambda)}{\lambda} \mathrm{d}\lambda. \qquad \mathbb{E}(\Lambda) = \int_0^{\infty} \lambda h(\lambda) \mathrm{d}\lambda$$

- $f_A$: The pdf (probability density function) of the observed 2D section profile areas.
- $g$: The pdf associated with areas of random sections of the reference particle. It is defined on the interval $(0, a_{max})$.
- $h$: The pdf of the diameters of the 3D particles.

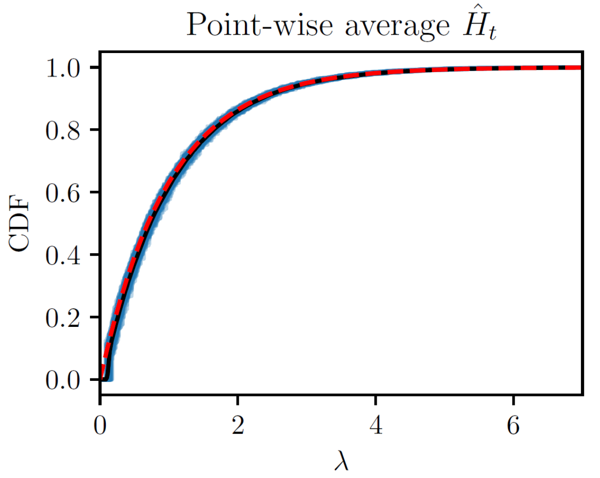
# Approach for estimating size distributions

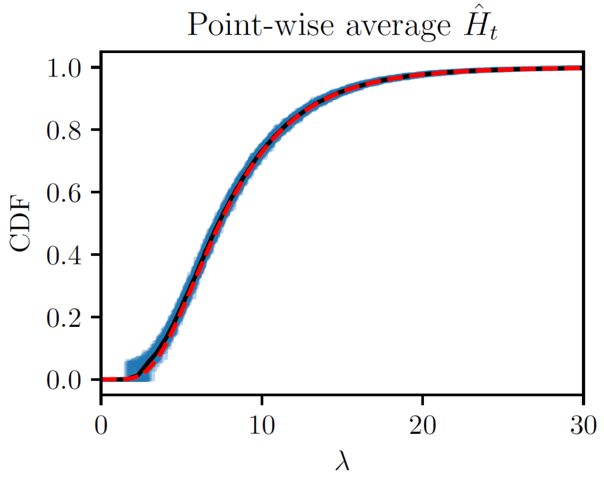
- We choose to estimate the Cumulative Distribution Function (CDF), of the particle volume distribution.
- We do not assume it belongs to a particular parametric family, e.g. lognormal distribution.
- The procedure may be summarized in two steps:

1. Estimate the biased volume distribution, by maximizing the log-likelihood.
2. De-bias this estimate to obtain an estimate of the volume distribution.

# Simulation results

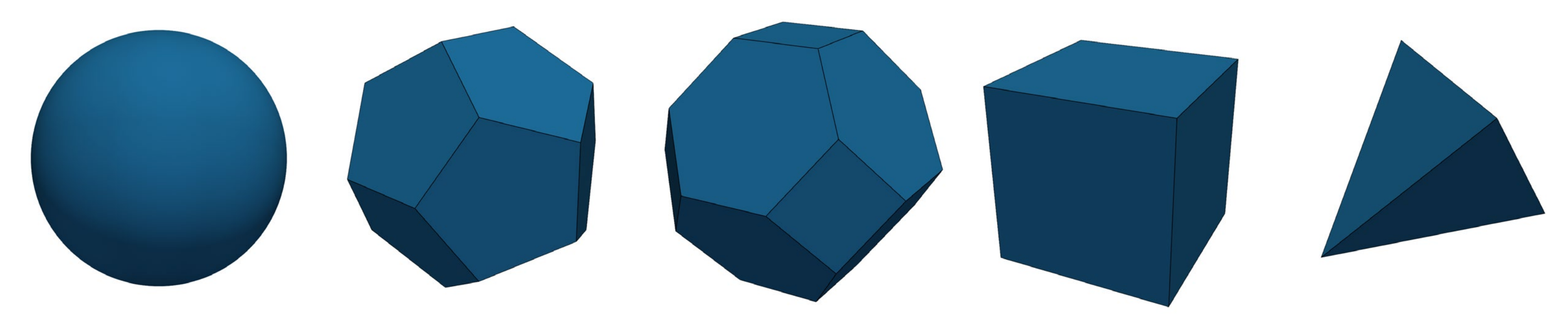
- We generate a sample of observed section areas, for a convex shape of choice, and a diameter distribution of choice.
- Shape: dodecahedron. Diameter distribution: on the left an exponential distribution, on the right a lognormal distribution.
- $n = 10000$, averaged over 100 repetitions.



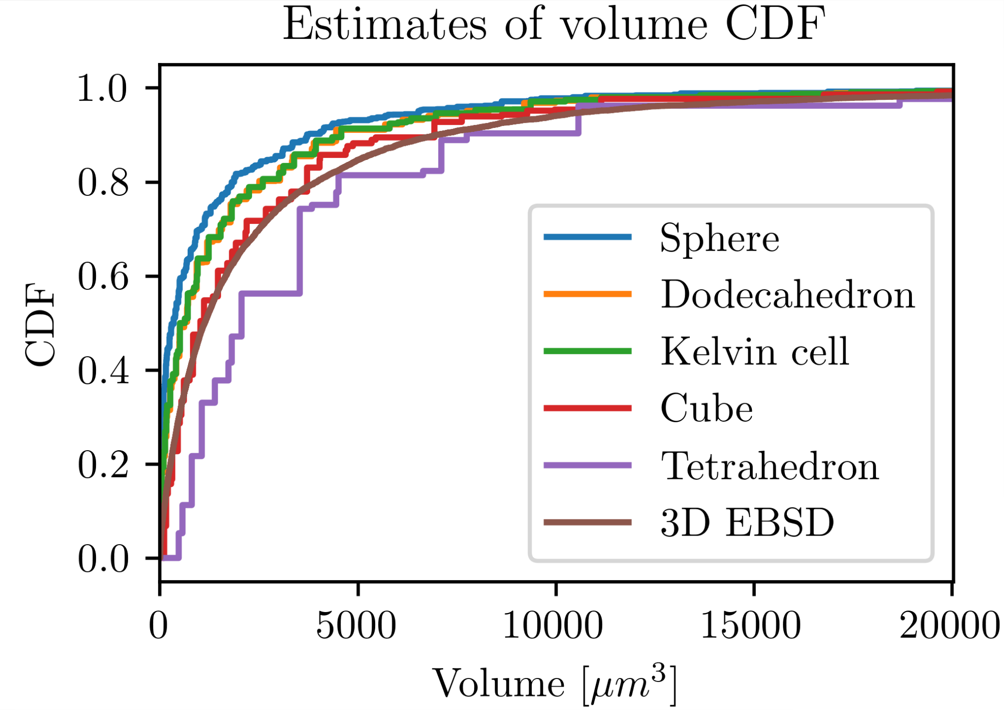
# Application to real data

- Material: Interstitial Free (IF) steel.
- 2D EBSD: 1506 observed grains, on the steel sheet surface.
- 3D EBSD: 9211 observed grains.
- We take the observed grain areas in the 2D EBSD, and estimate the grain volume distribution for various choices of convex shapes.



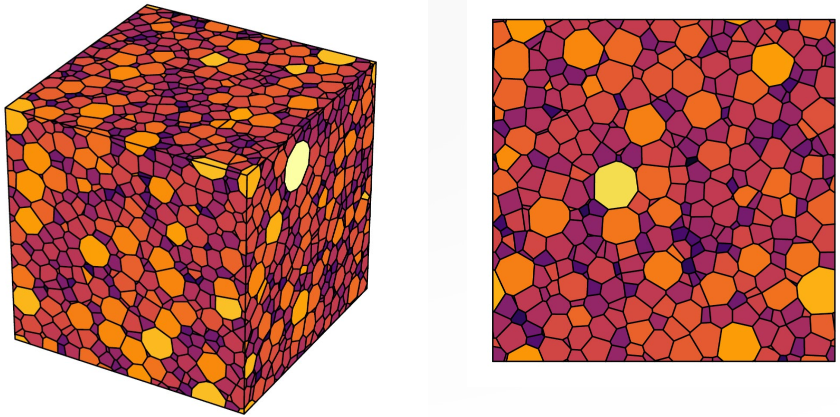
# Application to real data

- Promising results, especially for cubic particles



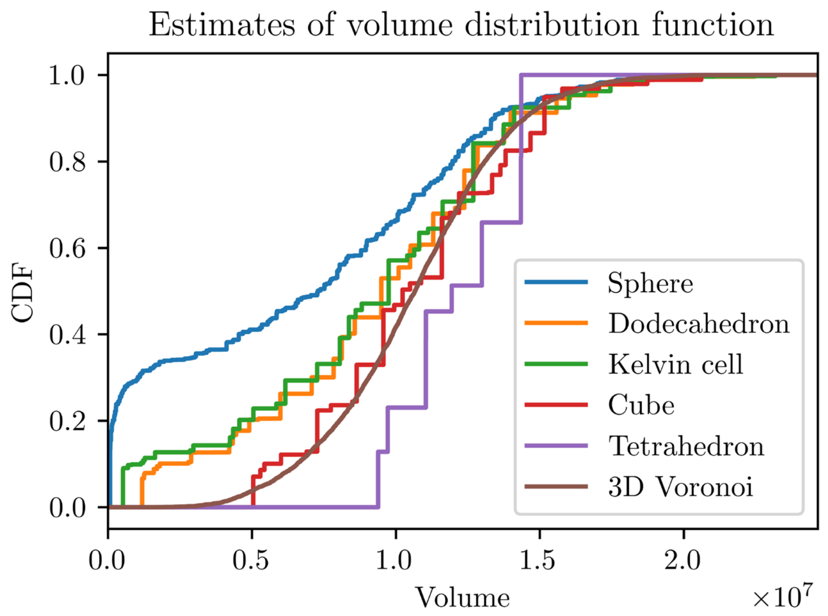
# Application to virtual microstructures

- A popular approach for modelling polycrystalline microstructures is via (Laguerre) Voronoi diagrams
- Simulation setting: generate a (Laguerre) Voronoi diagram and estimate the volume distribution of its grains using observed section areas.



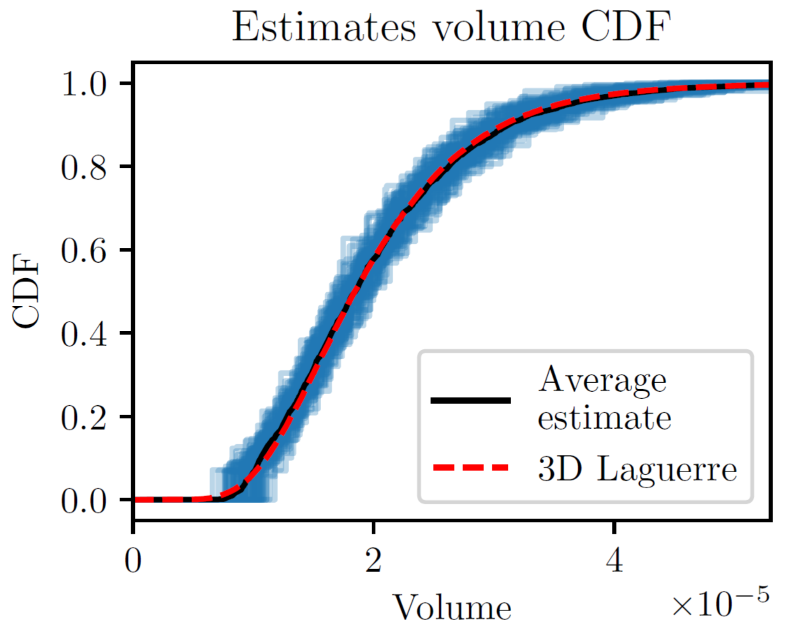
# Application to virtual microstructures

- A single Voronoi diagram was generated, its grain volume distribution estimated by combining the observed areas from 6 parallel sections.



# Application to virtual microstructures

- We perform 100 repeated simulations. This yields 100 estimates, each one corresponding to a different sample from 1 section of a Laguerre diagram.
- Shape: cube.



# Currently in progress

- More applications to real data.
- Application to virtual microstructures, such as (Laguerre) Voronoi diagrams.
- Can we explain why the cube works so well?

# Conclusions

- Via a mathematical model for randomly distributed particles we have derived a method for estimating grain size distributions.
- In the resolution of the problem we have addressed most of the formal mathematical challenges, and application to real data shows promising results.
- We are still working on further application to real data and virtual microstructures.

# Thank you

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