Virtual 3D microstructures with specified characteristics of state variable distributions

Edgar Gomes[1], Kim Verbeken[1], and Leo Kestens[1,2]

[1]Ghent University,
Department of Materials Science and Engineering
[2]Delft University of Technology,
Materials Science and Engineering Department

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Outline

Introduction

Framework

Grains

Texture

Results

Final words

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Physical model

is “a representation of the essential aspects of an existing system (or a system to be constructed) which presents knowledge of that system in usable form”[a]

[a] *Eykhoff*, System Identification: Parameter and State Estimation (1974).

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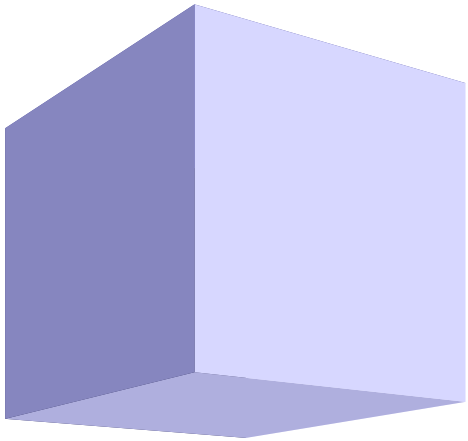
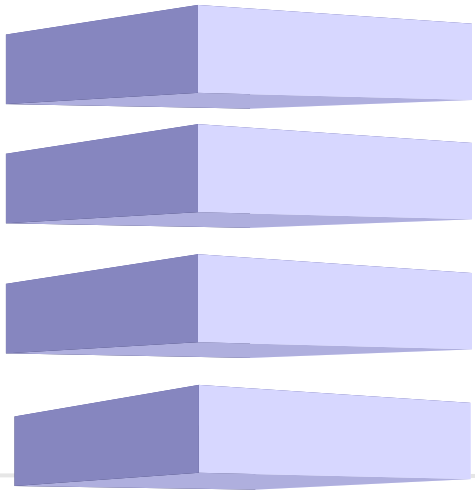
Motivation

3D measurements

of real materials are possible but consume relatively high amount of financial and time resources. Which implies in volume/statistics limitation.





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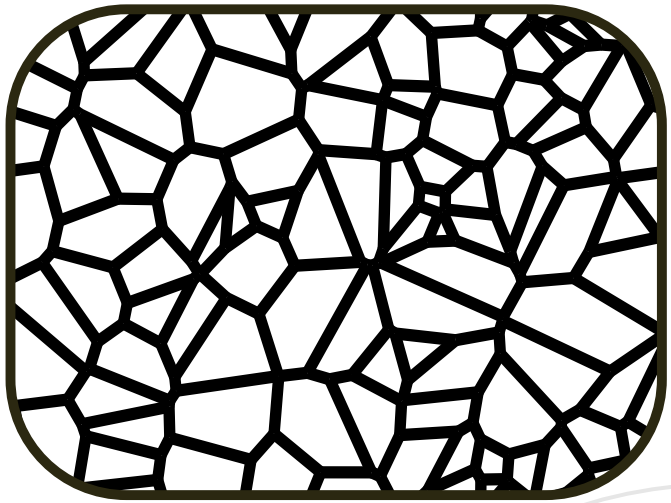
Virtual Materials

Virtual material

is an abstraction that represents characteristics of a microstructure in a computer data structure.



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1010101010
1010010101
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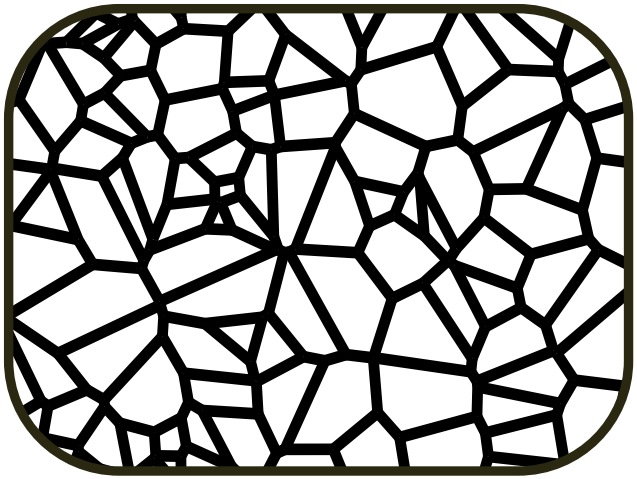
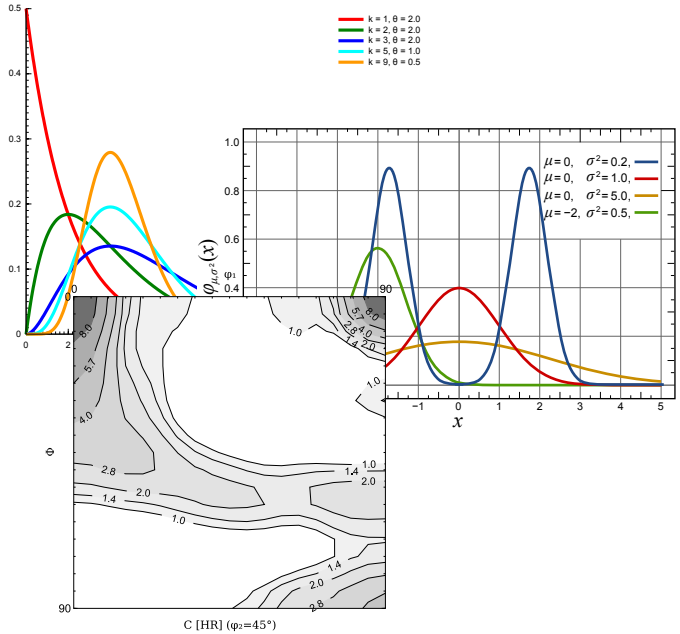
In the past decades ...





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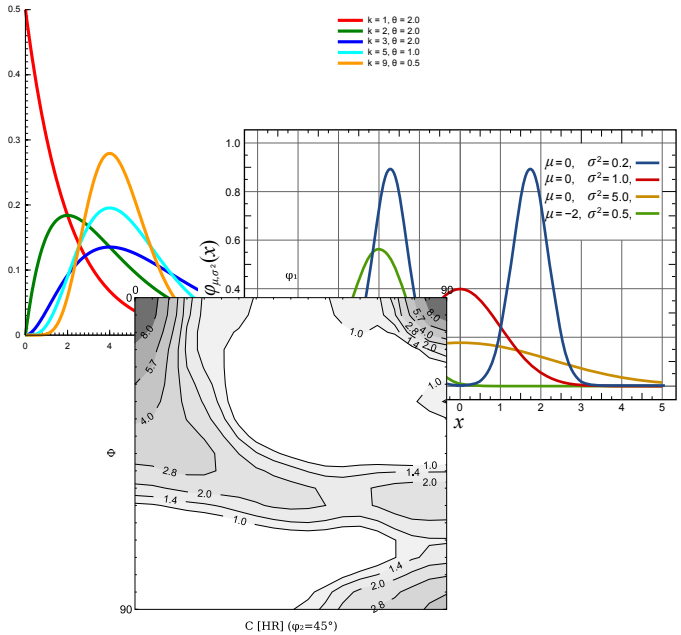
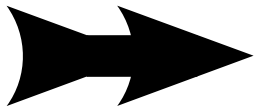
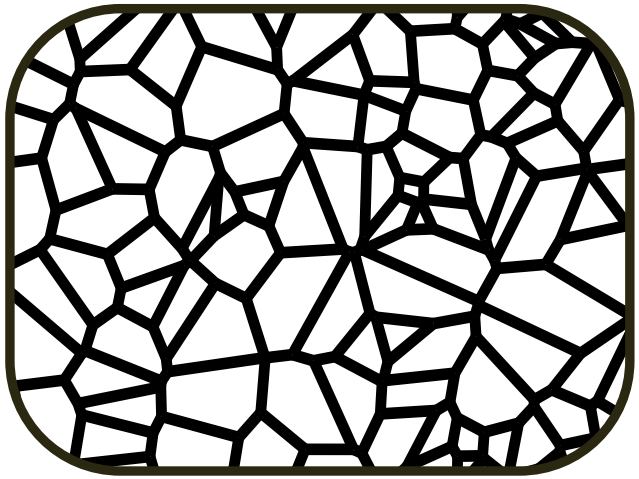
... but now we want the reverse!







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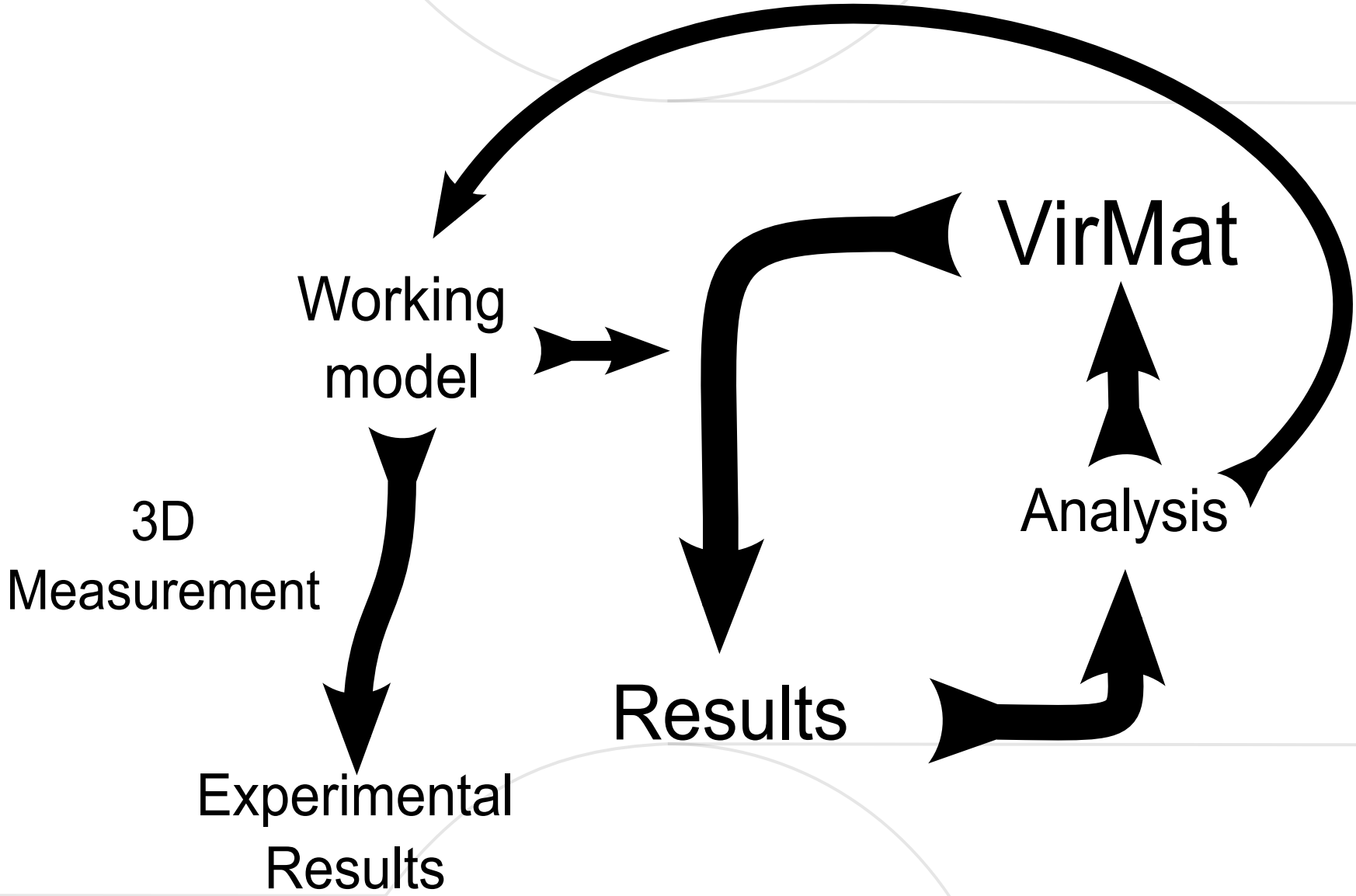
Our Solution



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Grain Morphology

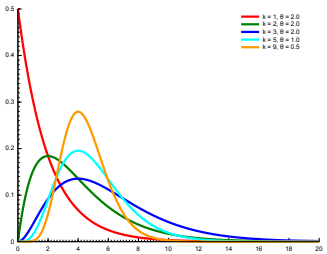
shape distribution

number of neighbours

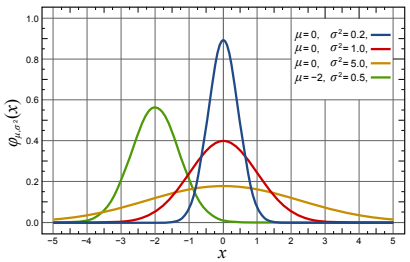
size distribution

clustering

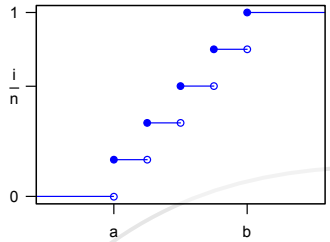
log-normal



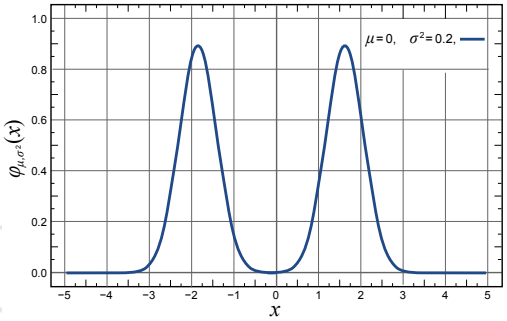
normal



discrete or custom



bimodal



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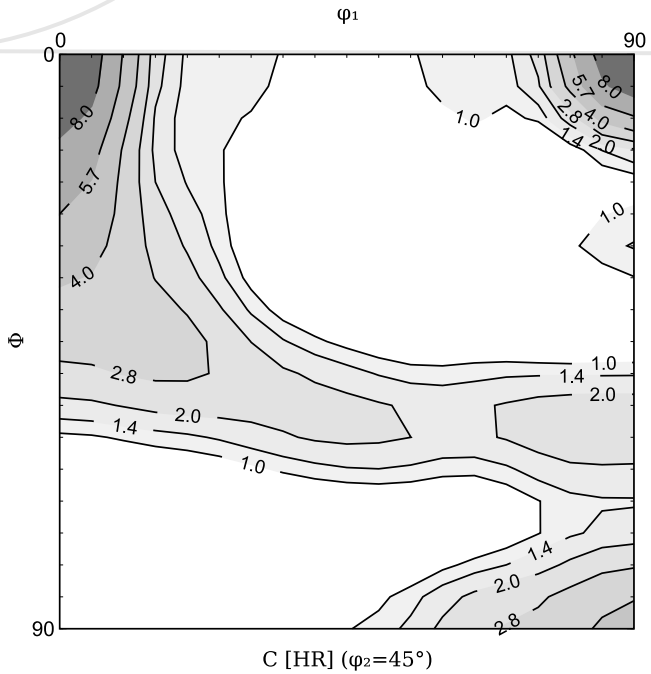
Texture

Orietation distribution

$$\frac{dV}{V} = f(g)dg$$

$$\oint f(g)dg = 1$$



$$f(g) = \sum_{l=0}^{\infty} \sum_{m=-1}^{l} \sum_{n=-1}^{l} C_l^{mn} \cdot T_l^{mn}(g)$$

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At first glance, both *Grain Morphology and Texture*, are independent ....

... but:

1. volume fraction constraint is implicit
   - no random texture with 2 grains
2. and...

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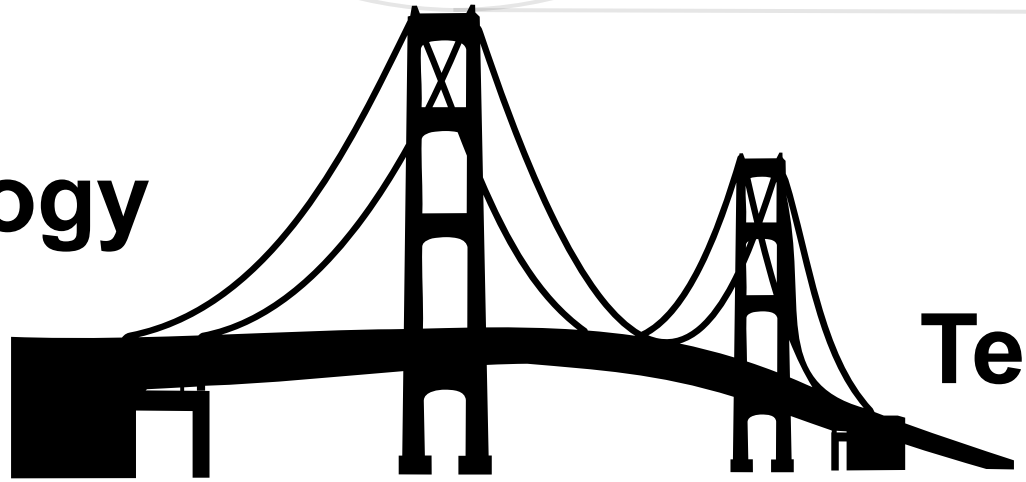
Grain Morphology



Texture

Grain Boundary Character Distribution

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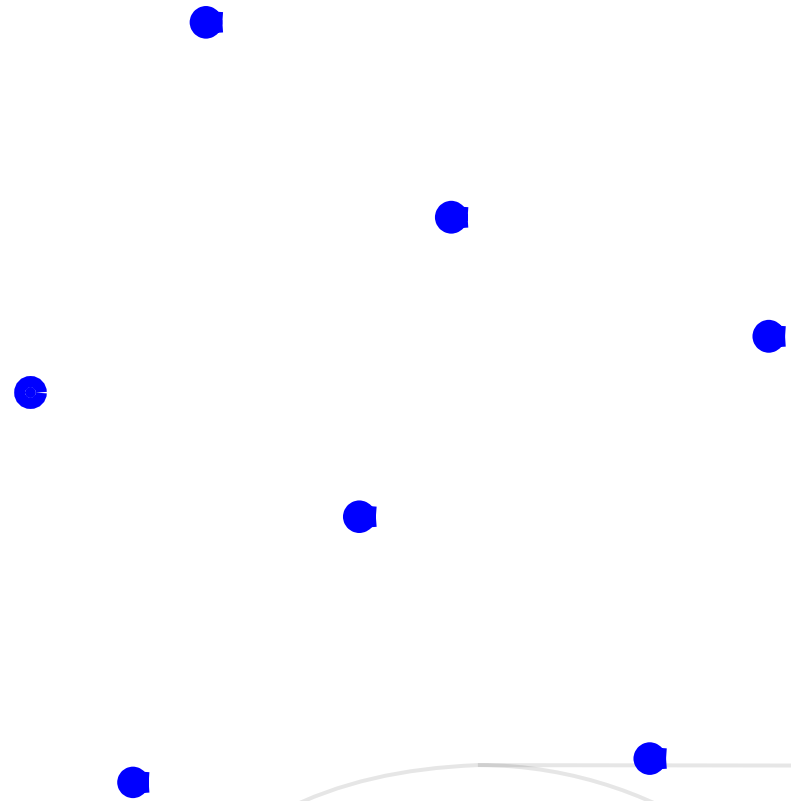
Space Partition



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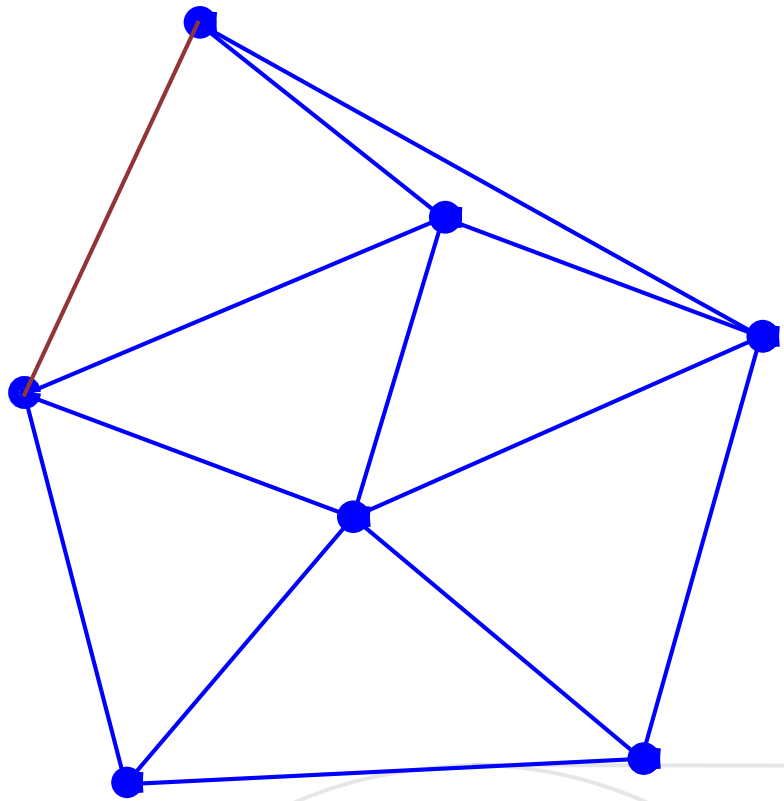
Space Partition



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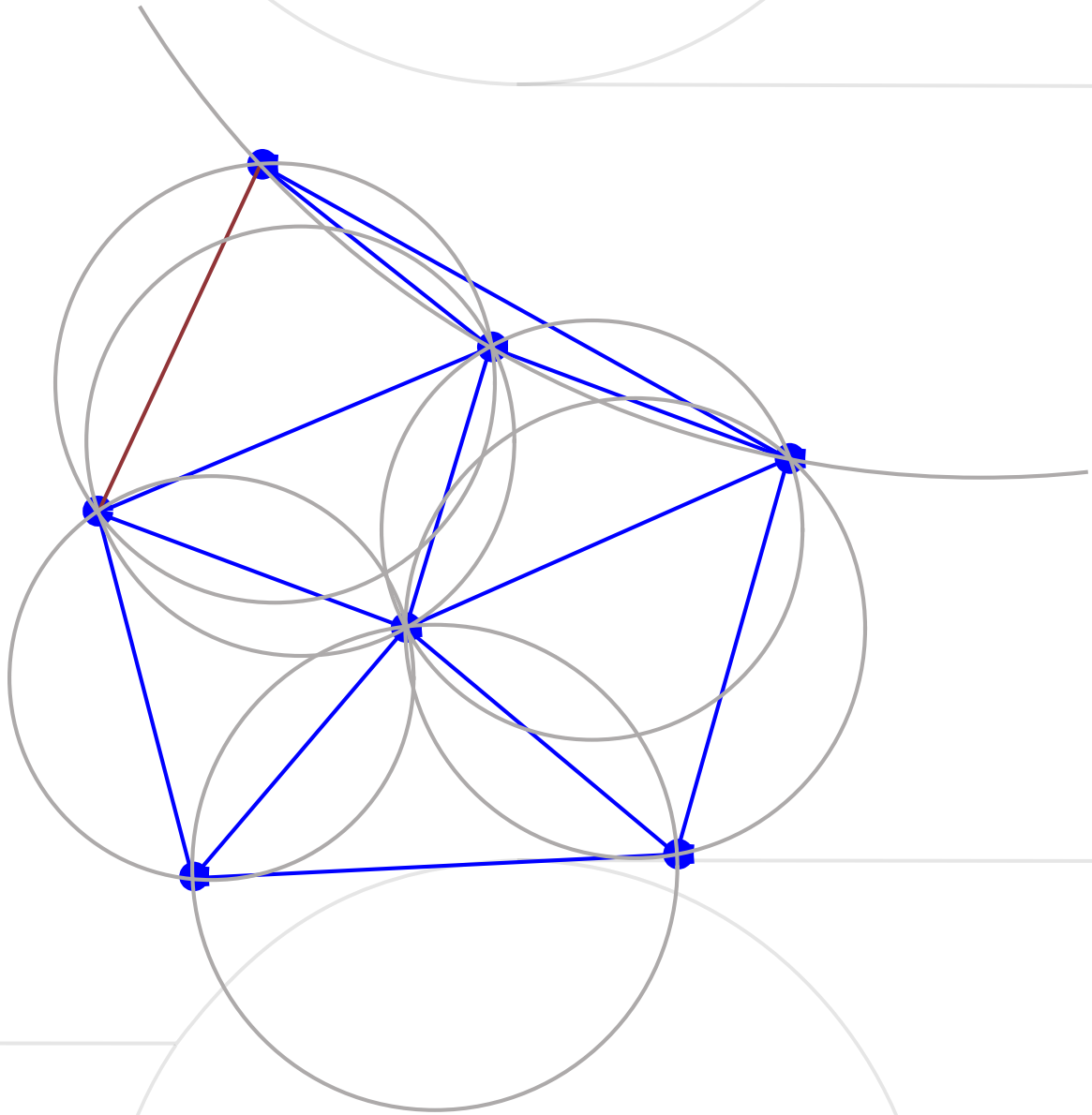
Space Partition



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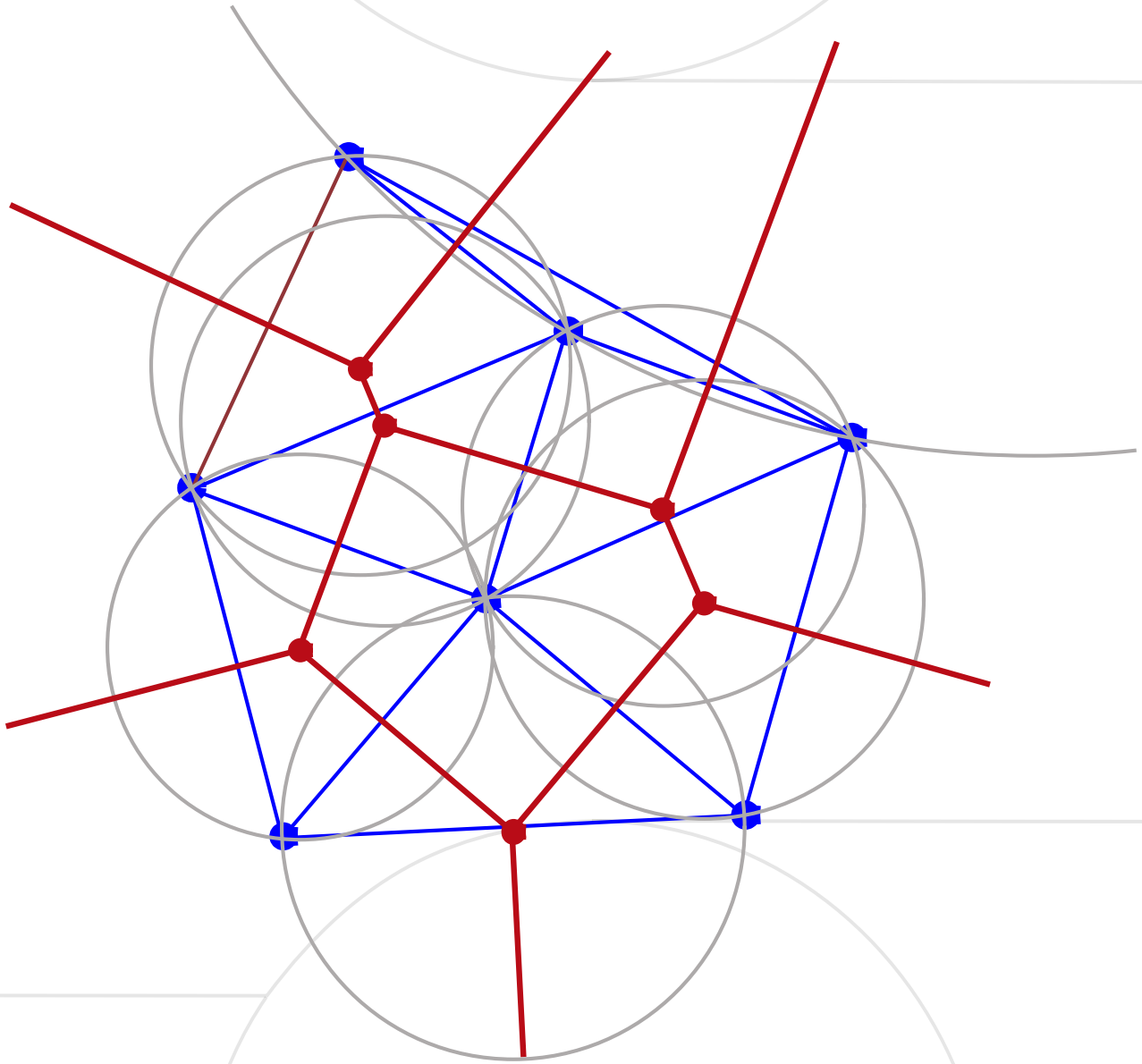

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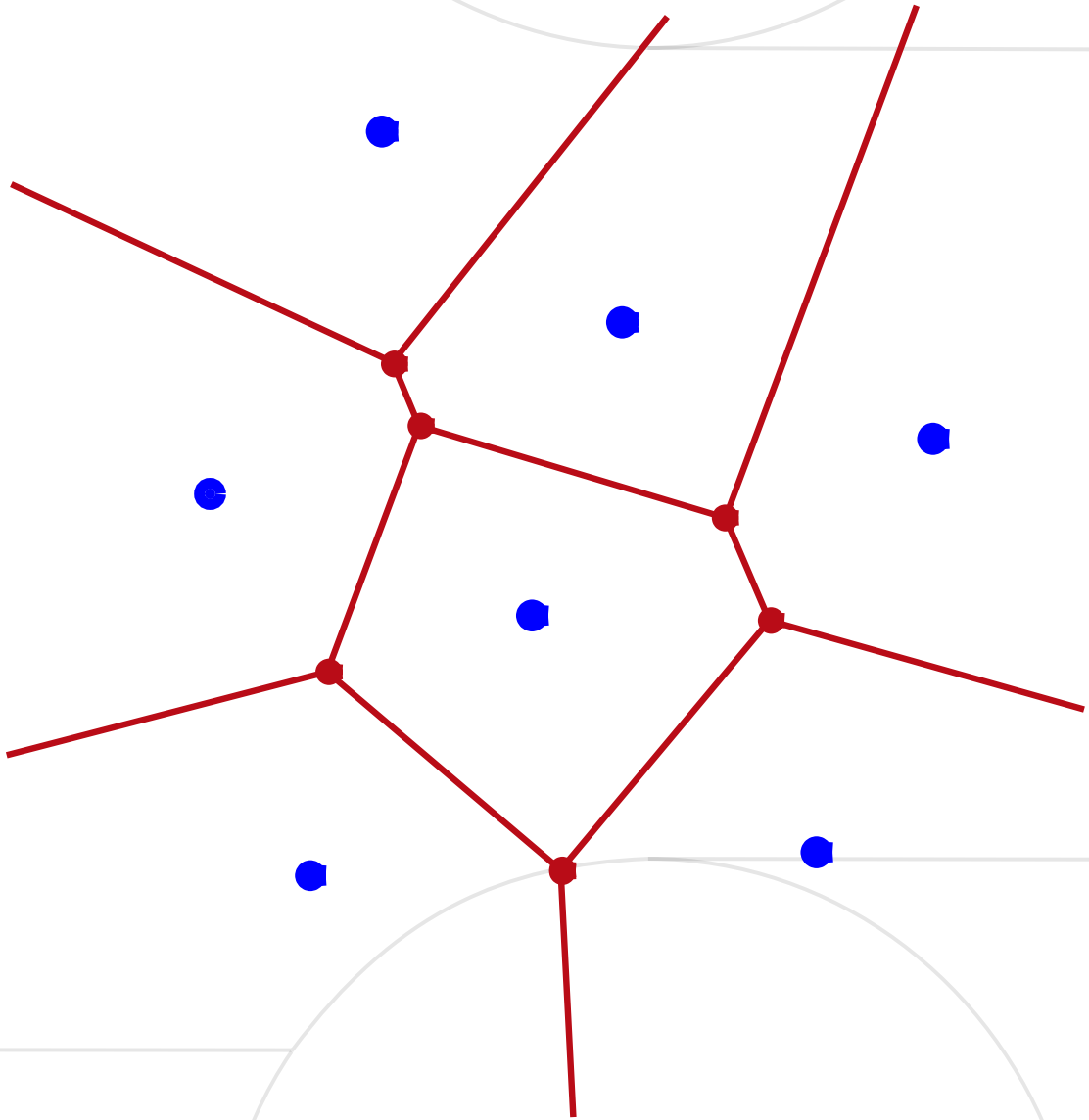

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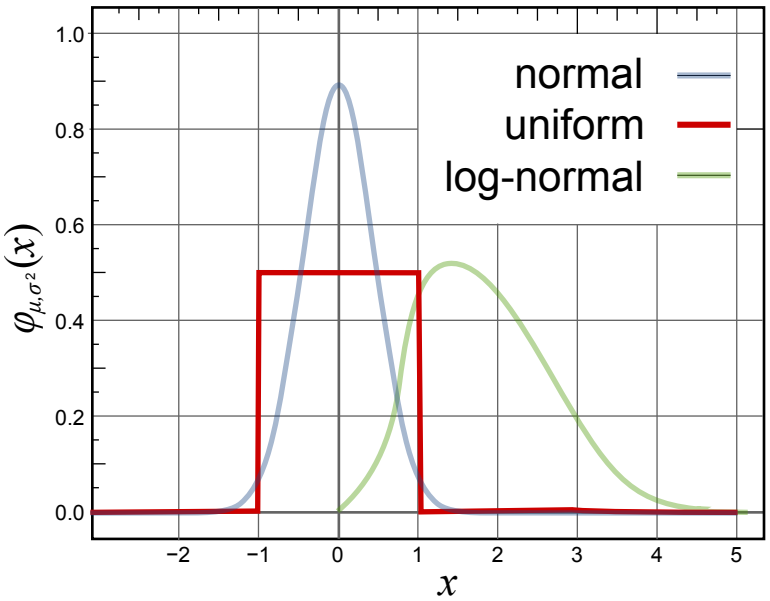
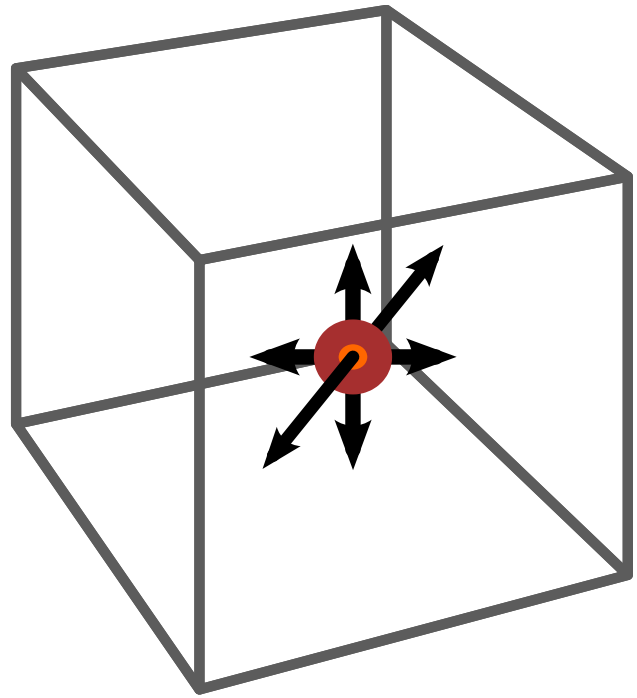
Uniform Random distribution





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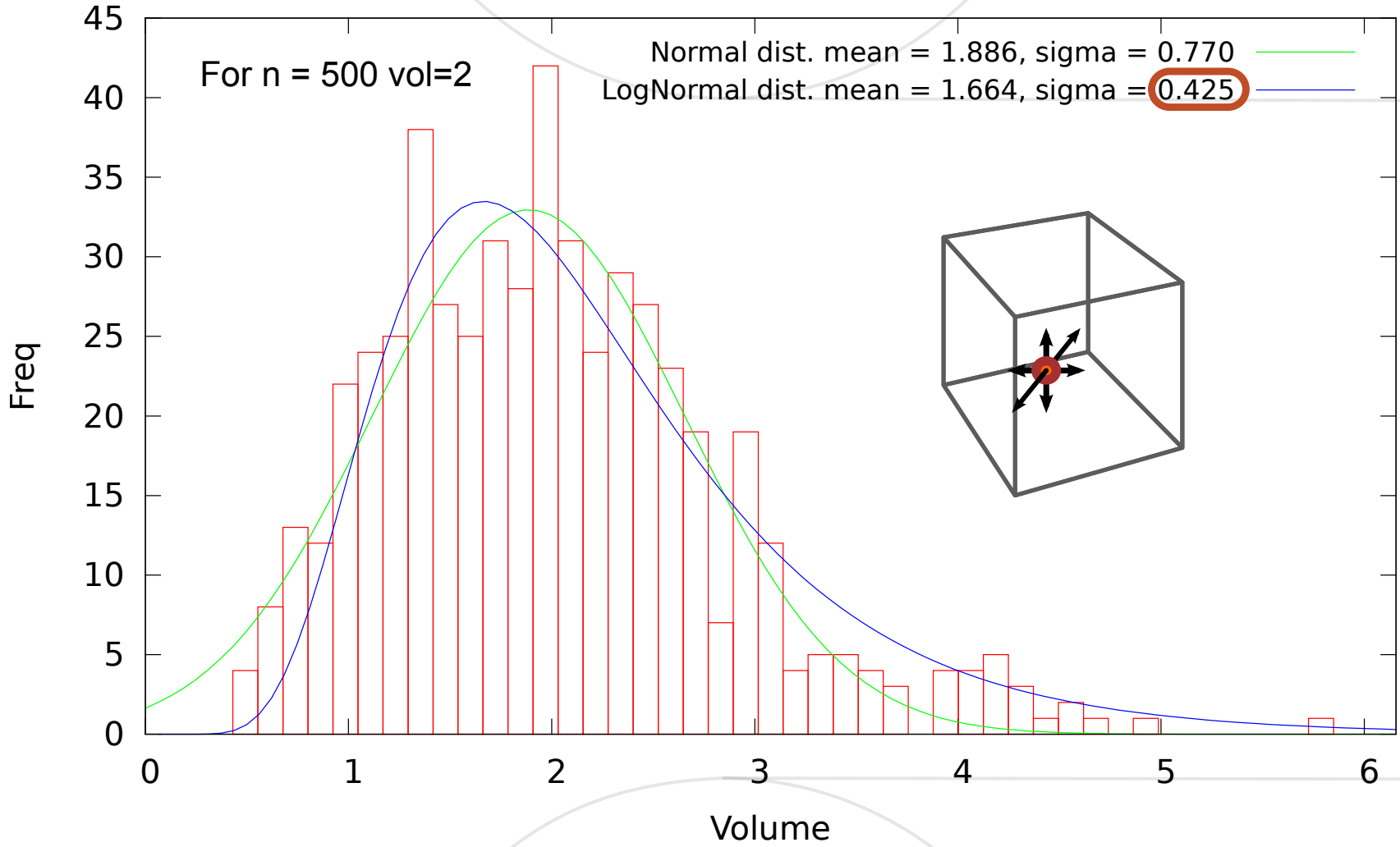

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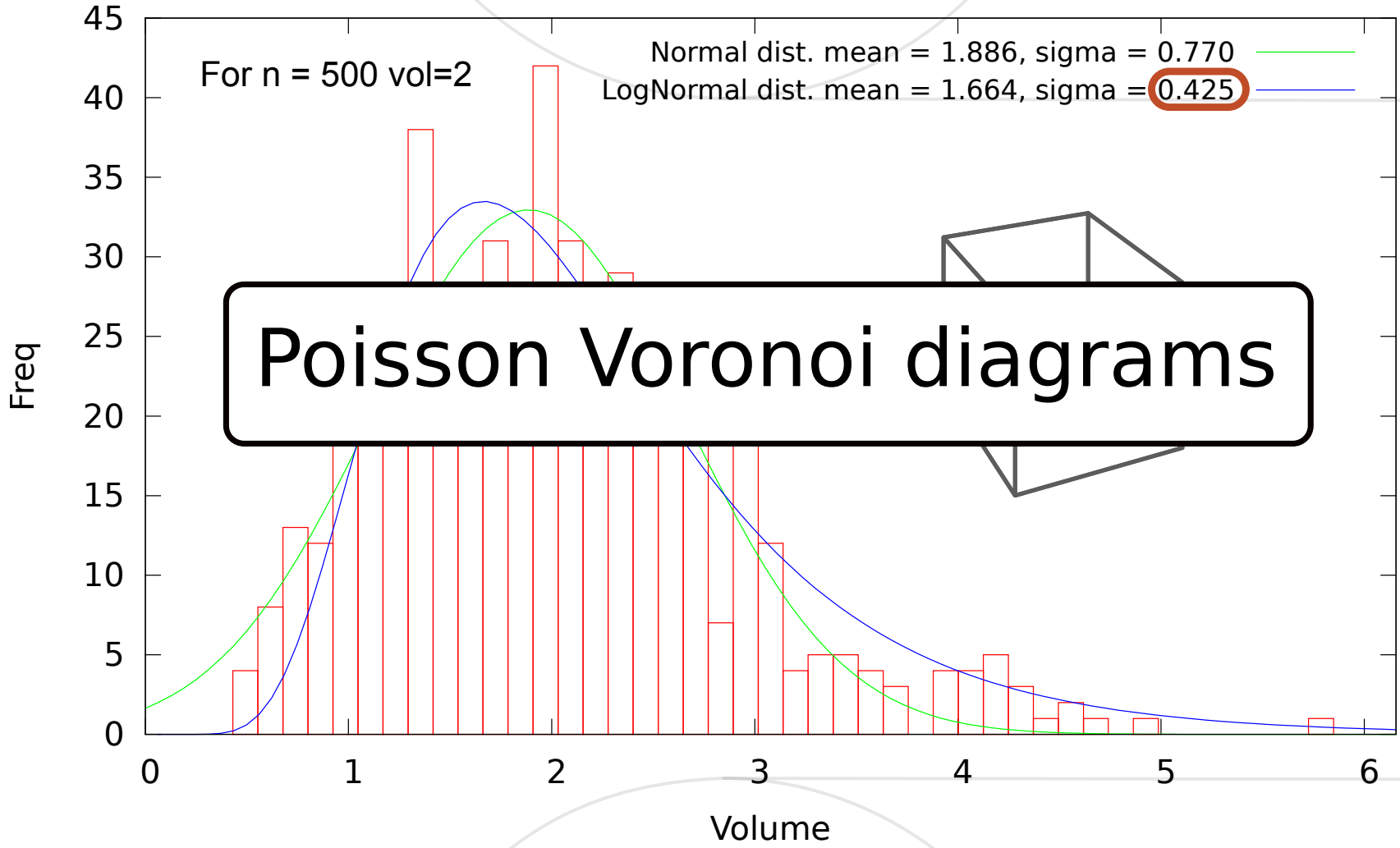

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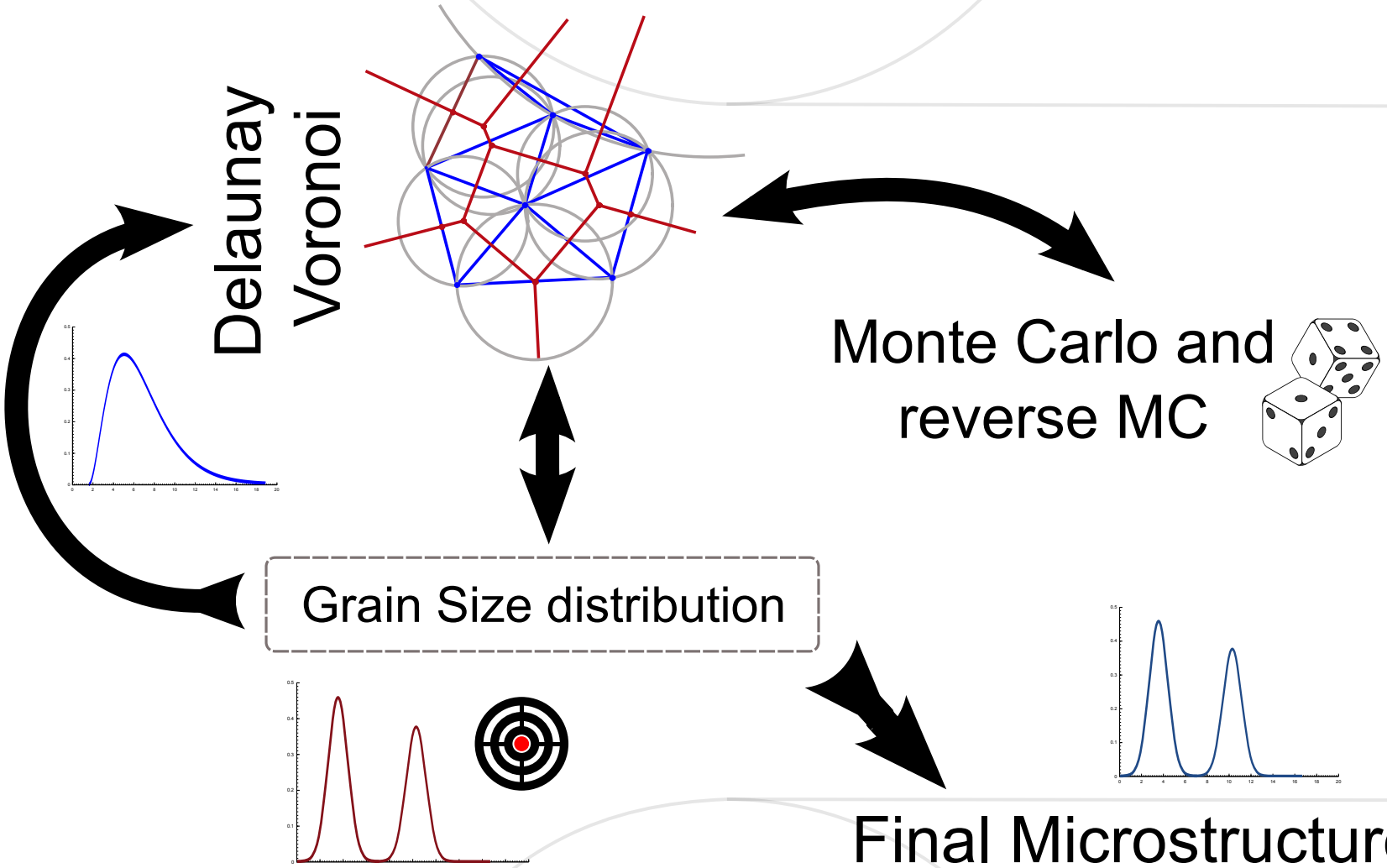

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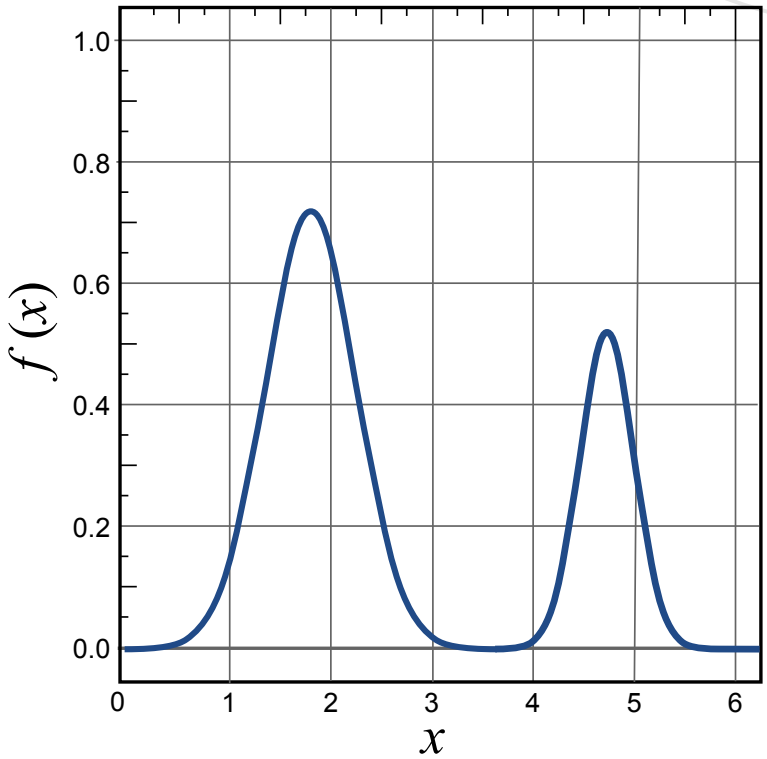
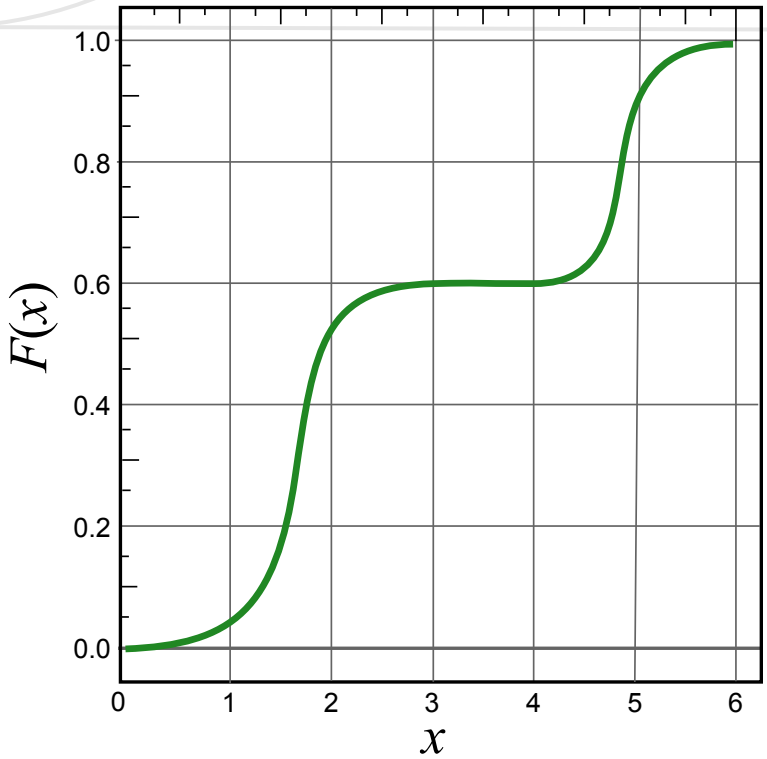
Orientation sampling





$$F(x) = \int_{-\infty}^{x} f(t)\, dt$$

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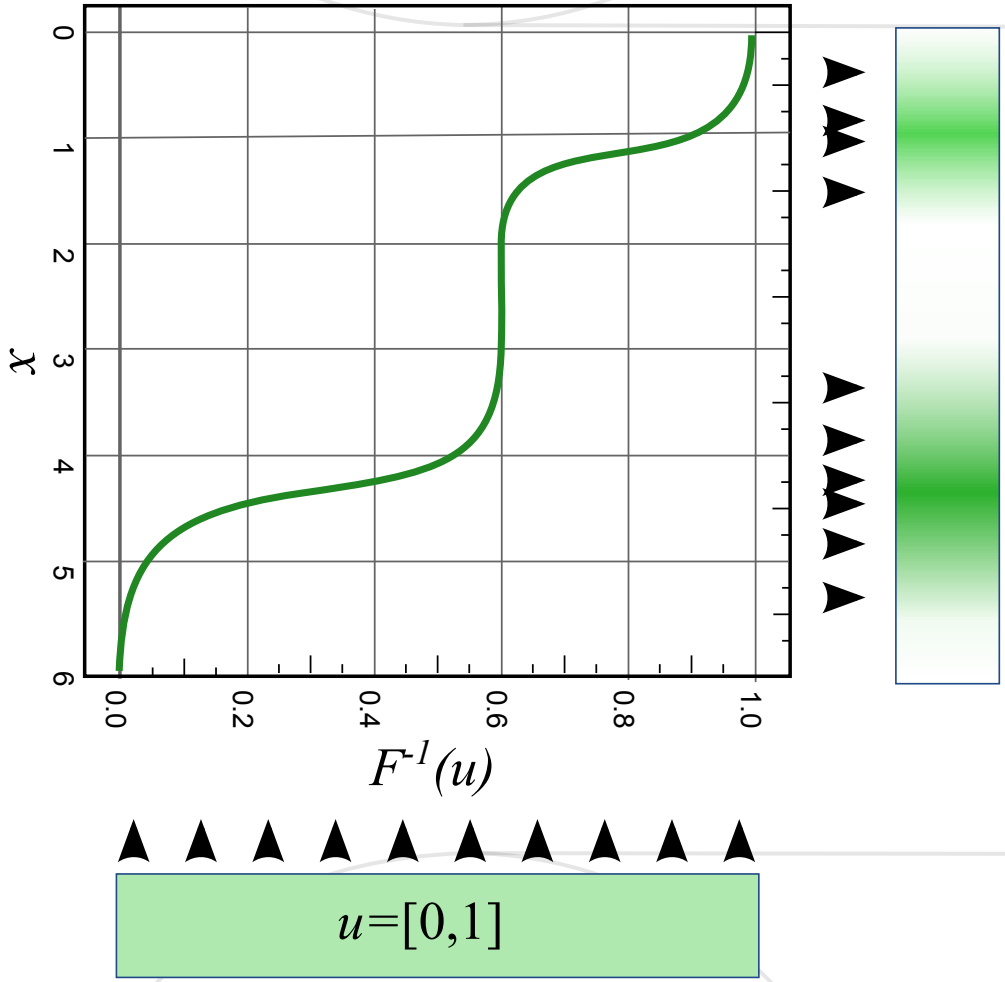
Orientation sampling



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Atention

sampling an ODF return values unrelated with the grain size distribution.

All sampled values are valid for constant grain size.

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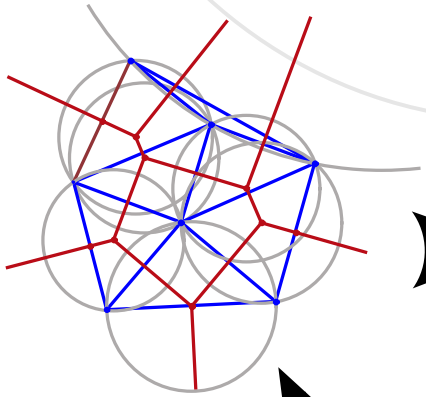
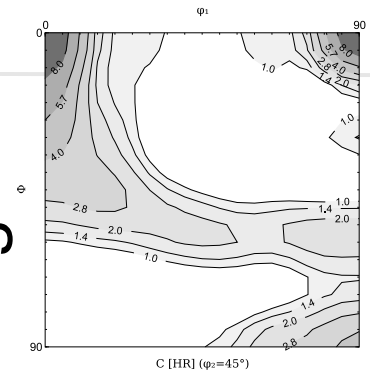
Delaunay
Voronoi



Orietation assignment

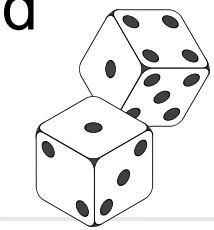


Grain Size distribution

Orientation distribution

Microstructure refinement

Monte Carlo and reverse MC



Final Microstructure

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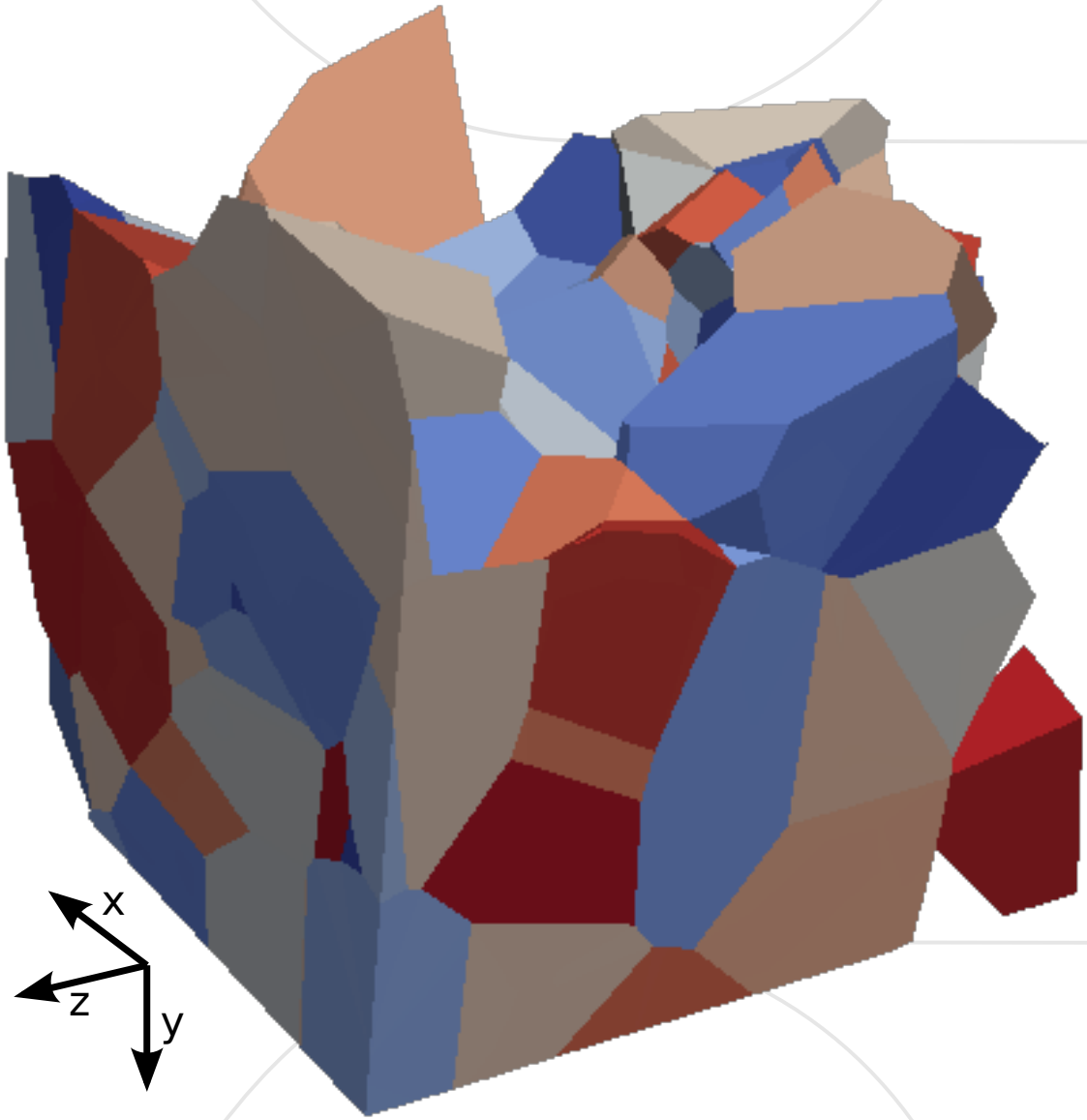
Grain Morphology



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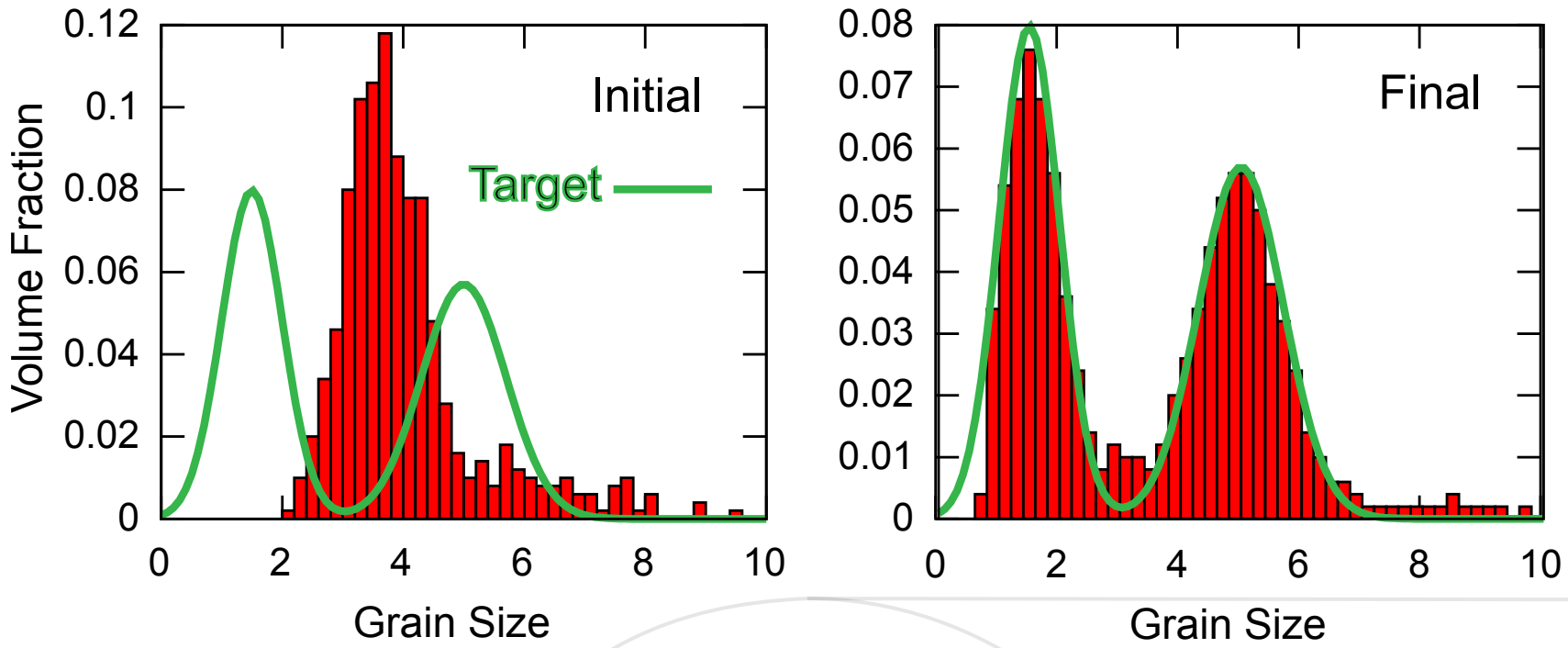
Grain Size Distribution

Histogram



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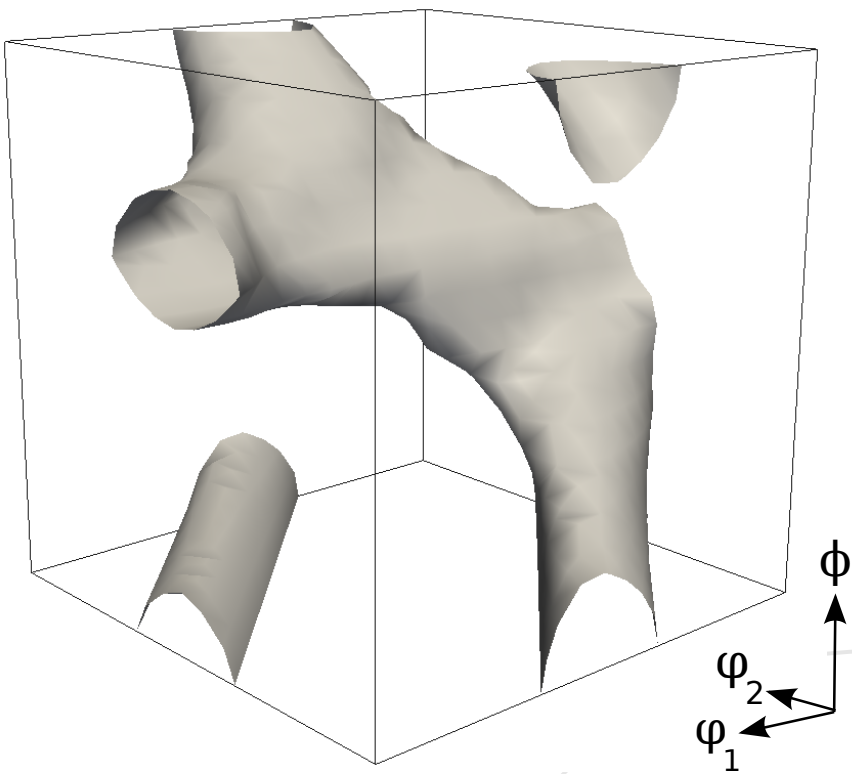
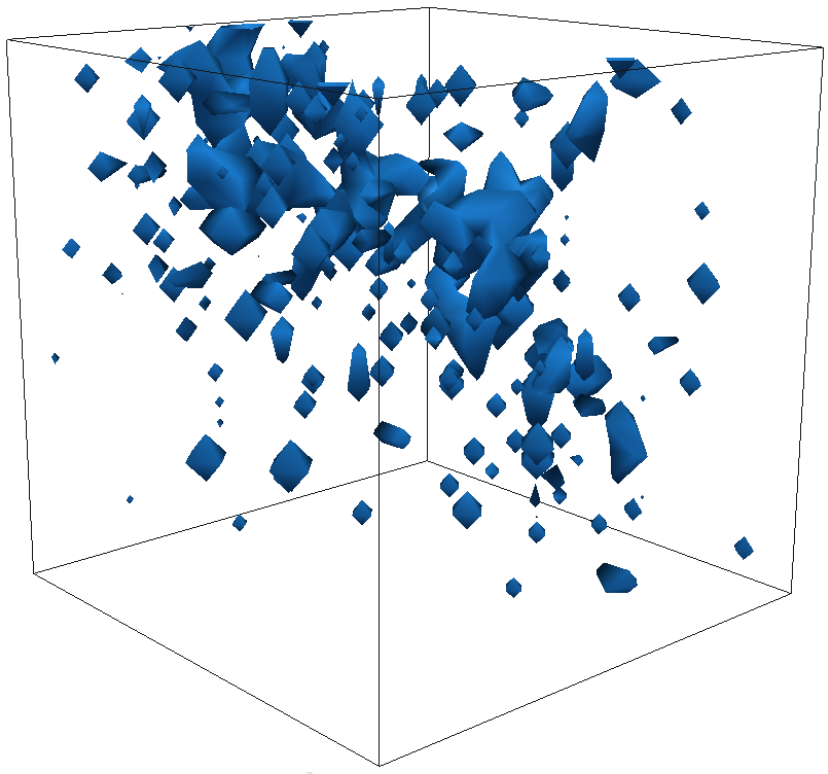
Orientation Distribution

Target

Initial sampling





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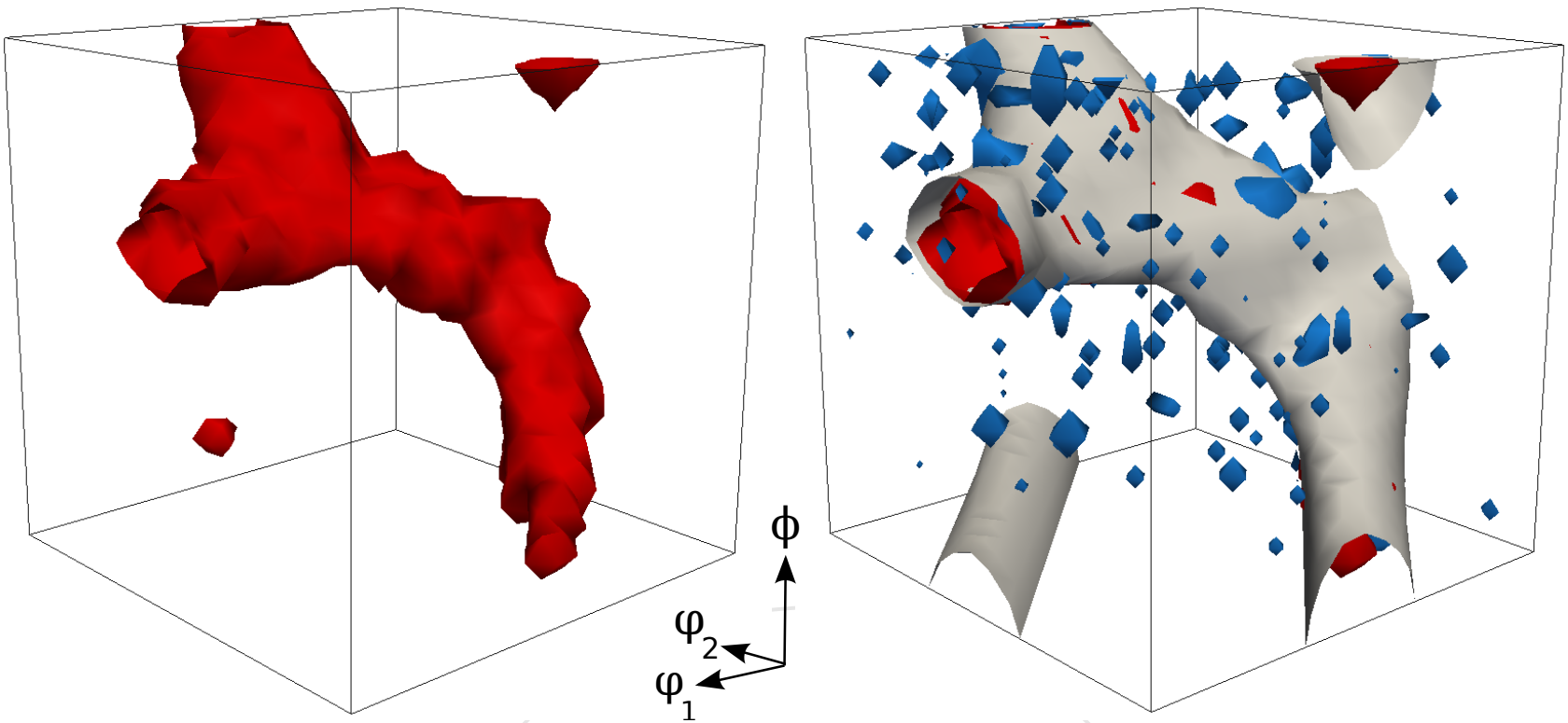
Orientation Distribution

Final



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Future work

1. Faster algorithm for grain generation with control of others properties other than size distribution.
2. Sampling orientations regarding grain size distribution.
3. Merge distributions into a high dimension distribution function (DF).
4. Sampling set of properties from high dimensions DF.

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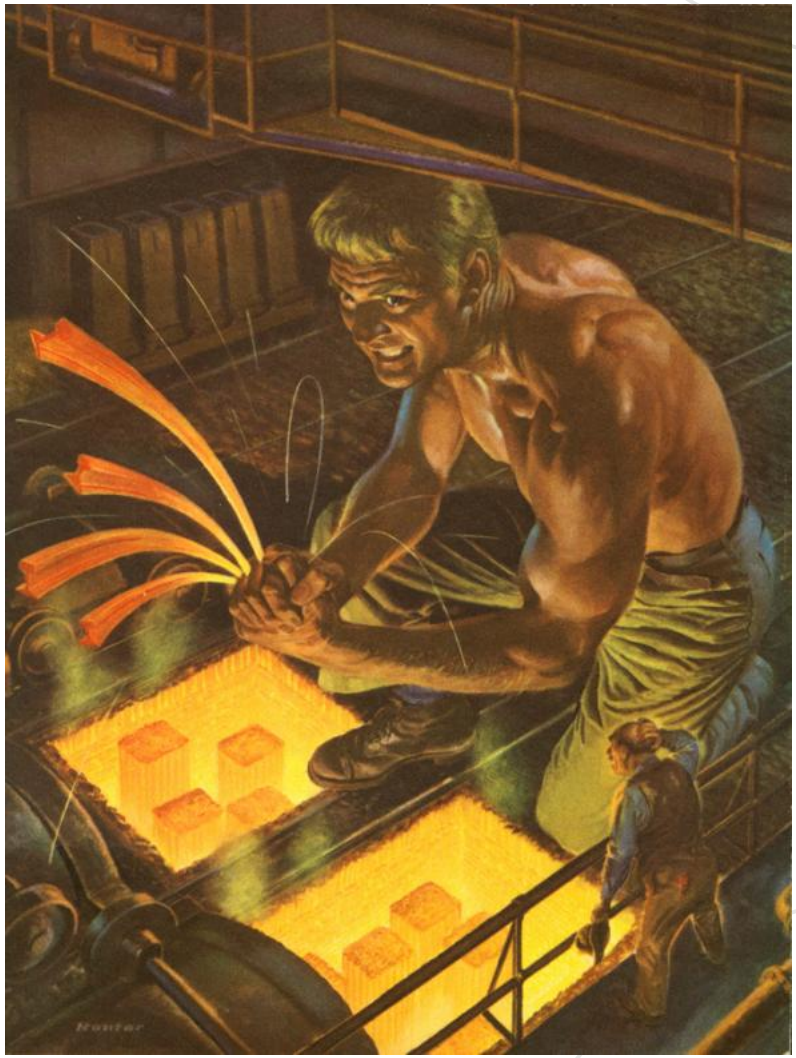
Thank for your attention !!!



"Joe Magarac was an imaginary folk hero whose story came from eastern European immigrants working in Pittsburgh area steel mills. His physical power and his brave, generous, and hard-working character made Joe Magarac (whose name "Magarac" means "donkey" in Croatian) the greatest steelworker who ever lived." [a]

Edgar.Gomes@UGent.be

[a] *http://www.jaha.org/edu/discovery_center/work/folk_hero.html*