

# Generalized Voronoi Diagrams and Applications

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## Abstract

This report documents the program and the outcomes of Dagstuhl Seminar 25492 “Generalized Voronoi Diagrams and Applications”, which was held from 30 November to 5 December 2025. The seminar brought together 28 scientists working on various aspects of generalized Voronoi diagrams such as efficient diagram computation, fitting diagrams to observed cell systems or using Voronoi diagrams to model material microstructure. The report contains the abstracts of the tutorials and presentations held during the seminar. It also contains a summary of the discussion sessions that were organized in smaller break-out groups.

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## 1 Executive Summary

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## Motivation

Voronoi diagrams are fundamental geometric structures that divide space into regions based on proximity to points or sites. They play an important role in many fields of science and have become cornerstones of disciplines such as computational geometry, scientific computing, and optimization.

At the heart of this seminar are generalized Voronoi diagrams, with a primary focus on Laguerre diagrams and their rather recent generalizations – anisotropic power diagrams and generalized balanced power diagrams – which introduce piecewise quadratic cell boundaries, enabling more precise modeling of complex structures. Recently these diagrams have drawn significant interest from the materials science community for their remarkable ability to

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\* Editor / Organizer



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accurately depict the inner structures of polycrystalline materials, such as metals, ceramics, and rocks, offering valuable insights into their composition and properties. Due to their ability to follow more complex boundary structures, they are also of emerging interest in Voronoi-based image processing applications, e.g., in superpixel generation and image segmentation.

Current methods for computing generalized Voronoi diagrams from imaging data are limited to moderately sized diagrams comprising of about 1,000-10,000 regions. To handle large data sets enabling computations at high resolution, large sample size, and multiple time steps, it is vital to develop efficient algorithms. However, the research communities behind the algorithm development, geometric clustering, optimal transport, stochastic geometry, and computational geometry are largely disjoint, with each field relying on different mathematical foundations and techniques. Applications such as the modelling of materials microstructures by Voronoi diagrams present yet another set of challenges for diagram calculations. Examples are the statistical fitting of models to observed data, fitting for incomplete data where only partial information of the cell system is observed, and handling of material inhomogeneities and edge effects.

The goal of this Dagstuhl Seminar was to bring together leading researchers from the diverse mathematical areas and materials scientists to learn from each other, spark vibrant discussions, identify common grounds, advance their fields, and set the path for successful collaborations towards developing fast and robust generalized Voronoi diagram algorithms addressing the needs of the practitioners working in imaging and microstructure modelling.

### Programme

The seminar began with 3-minute/1-slide introductions by all the participants, which was a great way to break the ice since the seminar brought together diverse communities, and a lot of the participants had not met before.

This was followed by five 1-hour tutorials (four on Monday and one on Tuesday) to establish a common language and introduce some basic notions from experimental and computational materials science (Henning F. Poulsen and Orkun Furat), discrete mathematics (Peter Gritzmann), optimal transport (Bruno Lévy), and stochastic geometry (Claudia Redenbach). In each tutorial we saw different applications of generalized Voronoi diagrams and different tools and results.

The tutorials were followed by short research talks (20-minute talks plus 10 minutes of questions and discussion). All participants were invited to speak.

In addition, there were two 2-hour discussion sessions (reports from the breakout groups can be found below) and a software demonstration session, where Romain Quey gave a demo of *Neper* and David Bourne gave a demo of the *SyntheticMic* GUI, which are both software packages for generating synthetic polycrystalline microstructures using Laguerre diagrams. Bruno Lévy gave a tutorial on his geometry-processing library *Geogram*.

In addition to the scientific programme, there was an 8-km hike on Wednesday afternoon and a piano recital by Piere Calka on Thursday evening.

### Outcomes

One of the immediate outcomes of the seminar was knowledge exchange between what had previously been quite disjoint communities (materials science, computational and stochastic geometry, discrete mathematics, and optimal transport theory). Another immediate outcome was the identification of several open problems including how to reconstruct a 3D micro-

structure (or diagram) from 2D slices, how to model grain growth using generalized Voronoi diagrams, and how to efficiently compute an analytic representation of anisotropic power diagrams. In addition, initial follow-up activities have already begun, including invitations for research talks and online discussions to develop specific problems identified during the seminar.

Regarding longer-term outcomes, we expect the collaborations initiated at the seminar to result in joint grant applications and research articles, and to stimulate further focused workshops and research visits.

Overall, we feel that this was a very successful seminar. This impression is confirmed by the survey filled in by the participants. We are grateful to Christian Jung for organizing and compiling the abstracts. On behalf of the participants, we would like to thank Dagstuhl for enabling us to hold the seminar at Schloss Dagstuhl, which was the ideal venue.

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### 3 Overview of Tutorials

#### 3.1 Introduction to artificial neural networks and their applications in structural analysis and modeling of polycrystalline materials

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A broad range of engineered as well as natural materials exhibit polycrystalline microstructures, i.e., they consist of a large number of crystals (also called grains) with different atomic lattice orientations arranged in a space-filling manner. The macroscopic (functional) properties of these materials are often strongly influenced by their internal grain architecture, typically observed in experimentally acquired 2D/3D microscopic image data.

Artificial neural networks (ANNs) have become powerful tools for extracting information from this type of image data: convolutional neural networks can segment grains in 2D/3D image data, which in turn facilitates subsequent analysis and modeling workflows [1]. Beyond segmentation, ANNs can be deployed as generative models. For example, generative adversarial networks (GANs) can synthesize image data that exhibits grain architectures that are similar to experimentally observed ones [2]. Such artificially generated microstructures can serve as input for further numerical simulations, enabling virtual materials testing and thereby reducing experimental effort. Moreover, generative approaches can help overcome the limitations of 2D imaging techniques by learning to generate 3D images of grain architectures that are consistent with 2D observations.

Besides representing grain architectures as discretized image data, grain architectures can also be described in a space-continuous manner using tessellation models, in particular, power diagrams. Such representations are advantageous, as they are typically defined by relatively few parameters. Methods from ANNs can contribute to this representational framework by enabling the efficient fitting of power diagrams to segmented image data [3]. In particular, by leveraging programming libraries that enable automatic differentiation, gradient-based optimization can be used to identify parameters of power diagrams that best approximate the grain architectures observed in image data. Beyond deterministic fitting, differentiable implementations of power diagrams enable ANN-guided generative modeling [4]. ANNs can be deployed to learn the probability distribution of power diagram parameters instead of directly learning the distribution of high-dimensional image data, which would be the common approach in conventional GAN-based modeling. The combination of power diagrams with ANNs, induces geometric regularization, as generated samples are constrained to physically reasonable morphologies by the chosen type of power diagram. In particular, this approach facilitates learning the probability distribution of 3D grain architectures from just a few 2D images, thereby reducing the need for costly and time-intensive 3D experimental characterization.

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### 3.2 Diagrams, Clustering, and Coresets – and the representation of polycrystals

*Peter Gritzmann (TU München, DE)*

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- Joint work of** Peter Gritzmann, Andreas Alpers, Maximilian Fiedler, Fabian Klemm
- Main reference** Andreas Alpers, Maximilian Fiedler, Peter Gritzmann, Fabian Klemm: “Turning Grain Maps into Diagrams”, *SIAM J. Imaging Sci.*, Vol. 16(1), pp. 223–249, 2023.  
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**URL** <https://doi.org/10.48550/ARXIV.2203.10864>

We give a brief account on diagrams with a view towards representing and analyzing polycrystalline materials. In particular, weight-constrained anisotropic clustering allows to compute diagram representations of polycrystals from data on the volume, center and moments of the grains which are available through tomographic measurements. Also we show the effect of coreset techniques for significantly accelerating the computations.

### 3.3 Optimal Transport: a new asset in the numerical analysis toolbox

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The Fast Fourier Transform (FFT) had a considerable impact in numerical analysis, by making it very easy to solve the Poisson equation, omnipresent in Physics. According to Yann Brenier’s intuition, the Monge-Ampère equation that characterizes Optimal Transport solutions can be considered as a non-linear version of the Poisson equation. The Monge-Ampère equation plays a role each time a least action principle is constrained by a conservation law, a very general configuration in Physics. This motivates the quest for an efficient Monge-Ampère solver, that could play a role similar to the FFT for this type of problems, as well as for some problems in modern Machine Learning. After a general introduction to the topic, I shall focus on a particular configurations (semi-discrete L2 transport), that involves some generalized Voronoi diagrams (Laguerre diagrams), and for which some specific algorithms (Kitagawa-Merigot-Thibert) can solve problems of very large scale (billions points).

### 3.4 Random tessellations

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**Main reference** Claudia Redenbach, Christian Jung: “Random Tessellations: An Overview of Models”, pp. 35–80, Springer Nature Switzerland, 2025.

**URL** [https://doi.org/10.1007/978-3-031-87264-8\\_2](https://doi.org/10.1007/978-3-031-87264-8_2)

Random tessellations are a prominent class of models in stochastic geometry. In our tutorial, the notion of a random tessellation and basic geometric characteristics of random tessellations are introduced. Several prominent model classes are presented: Voronoi tessellations and their weighted generalizations, hyperplane tessellations, and STIT tessellations. Some statistical methods and applications are also discussed.

## 4 Overview of Talks

### 4.1 PyAPD: A Python library for working with minimisation diagrams with GPU acceleration

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**Joint work of** Maciej Buze, Jean Feydy, Steven M. Roper, Karo Sedighiani, David P. Bourne

Minimisation diagrams, such as Voronoi tessellations, play a pivotal role across science and engineering, with applications ranging from modelling biological and chemical structures to mesh generation for finite element methods [1] and nearest-neighbour searches [2]. They have strong theoretical ties to optimal transport [3] and can be fitted to data using logistic regression, which underpins a lot of modern machine learning methodology [4].

In my talk I will present PyAPD [5], a Python library for working with minimisation diagrams, which leverages a specialised GPU-oriented library for symbolic kernel operations (KeOps [6]) to achieve near instantaneous computation of a generic large minimisation diagram (a 3-4 orders of magnitude speed-up versus baseline GPU (PyTorch) and CPU (NumPy) implementations).

In particular, I will showcase the capabilities of the library in the context of microstructure modelling [7], discuss on-going extensions (unbalanced optimal transport and higher-order minimisation diagrams) and present ideas for collaboration enabled by the ideas underpinning PyAPD.

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## 4.2 A few asymptotic results for functionals of Poisson-Voronoi cells

Pierre Calka (*University of Rouen, FR*)

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Joint work of Pierre Calka, Aurélie Chapron, Nicolas Chenavier, Cecilia D’Errico, Yann Demichel, Nathanaël Enriquez

In this talk, we consider the classical model of a random Voronoi tessellation generated by the points of a Poisson point process and derive in various settings distributional properties or expectation estimates for several functionals of the cells.

When the underlying Poisson point process is homogeneous in the Euclidean space, we can define the notion of typical cell in the Palm meaning, which is equal in distribution to the Voronoi cell generated by a fixed deterministic nucleus added to the point process, see e.g. [7] or [8, Section 10.2].

It is easy to show that the law of the volume of the largest ball centered at the nucleus and included in the typical cell is exponential. The distribution of the maximal distance from a point in the cell to the nucleus is another matter. In a recent work [3], we obtain precise asymptotics for the distribution tail of that distance and deduce from it and from a previous work [2] the fact that the extremal index related to the sequence of such distances for all Voronoi cells included in a large box is equal to  $(2d)^{-1}$ .

In the setting of the two-dimensional Poisson-Voronoi tessellation conditioned on the event that the typical cell contains a fixed large shape, we derive asymptotics for the expectation of the defect volume, perimeter and number of vertices of the cell [5]. Moreover, in view of studying the neighboring cells with an elongated shape, we study a toy model where the Voronoi nuclei are located in the lower half-space and we obtain a limit shape result for the renormalized typical Poisson-Voronoi cell with fixed height [6].

In the setting of a Poisson-Voronoi tessellation along a Riemannian manifold, we study the Voronoi cell associated with a deterministic nucleus and show that when the intensity goes to infinity, the expectation of the number of vertices of the cell has a two-term expansion which involves the scalar curvature of the manifold at the nucleus point [1].

Finally, we present a model of iterated Voronoi tessellations introduced by S. Zuyev and K. Tchoumatchenko [9]. Inspired by their construction, we propose a planar toy model for a fractal random set which is based on a sequence of regular tessellations. We then provide explicit values for its box and Hausdorff dimensions [4].

In the process, we discuss a few open questions related to these topics.

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### 4.3 Overlay of Voronoi tessellations for lunar Euclidean MSTs

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Related or higher-order Voronoi tessellations, we consider the overlay of several order-1 Voronoi tessellations. These tessellations are motivated by the study of chromatic persistent homology and, in particular, the equivalence of the relative chromatic diagram and a more conventional diagram that analyzes the persistent growth pattern of lunes (which we define as intersections of equal-size balls).

### 4.4 CVT-based data-adaptive family of partitioning algorithms and materials modeling

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**Joint work of** Maria Emelianenko, Guy B. Oldaker, Katherine Saleme Ruiz, Dmitry Golovaty  
**Main reference** Maria Emelianenko, Guy B. Oldaker IV: “On the optimality of voronoi-based column selection”, Numerical Methods for Partial Differential Equations, Vol. 40(6), p. e23137, 2024.  
**URL** <https://doi.org/10.1002/num.23137>

In the first part of the talk, we present a unified family of data-adaptive partitioning algorithms that extends several well-known methods (e.g., k-means and k-subspaces) [1, 2]. Indexed by a single parameter and employing a common centroidal Voronoi tessellation-based minimization strategy, the algorithms are easy to use and interpret, and scale well to large, high-dimensional problems. The data-adaptive framework developed in this work: (a) exhibits skill at automatically uncovering data structures and problem parameters without any expert knowledge, (b) can be used to augment other existing methods. Analytical results and numerical experiments presented in this talk highlight the advantages of the new methodology in the context of several disparate application areas, including subspace clustering, model order reduction, and matrix approximation.

The second part highlights recent work on microstructure modeling in polycrystals, using large-scale curvature-driven grain growth simulations and mesoscopic formulations [3]. It is shown that microstructure entropy plays an important role both in the formation of grain boundary statistics as well as in the form of the elastic and plastic response. Stochastic modeling, including random walk descriptions, and applications to additive manufacturing microstructure characterization are presented.

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## 4.5 Provably Robust Perspective- $n$ -Point Algorithms for Camera Pose Estimation

Dan Feldman (*University of Haifa, IL*)

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In the Perspective- $n$ -Point problem (PnP), we are given a 2D image of a known 3D object that was captured by a pinhole camera, and the goal is to estimate the position of the camera. More formally, the input is a set of  $n$  points  $p_1, \dots, p_n$  in  $\mathbb{R}^3$ , and corresponding  $n$  lines  $\ell_1, \dots, \ell_n$ , where each line intersects the origin of  $\mathbb{R}^3$  (the pinhole). We wish to compute an alignment, i.e., a rotation matrix  $R \in \text{SO}(3)$  and a translation vector  $t \in \mathbb{R}^3$ , that minimizes some function  $f(\text{dist}(Rp_1 + t, \ell_1), \dots, \text{dist}(Rp_n + t, \ell_n))$  of the distances between each aligned point to its paired line. The Least-Mean-Square function  $f(\cdot) = \|\cdot\|_2^2$  is easier to compute, but sensitive to noise and outliers.

We suggest the first provably good approximation algorithms for the global optimum of robust versions of the PnP. These include: sum of (non-squared) distances  $f = \|\cdot\|_1$ ,  $M$ -estimators and  $m$ -outliers (where large distances have a bounded effect or are ignored, respectively). The expected running time is  $O(n \log n)$  for a sufficiently large  $n$ , and the multiplicative approximation factor is  $O(1)$  in the worst-case.

This is by providing a generic algorithm that minimizes any given log-Lipschitz function  $f$  of the distances. It forges novel links between objects in geometric topology, such as Clifford torus, optimization techniques from computational geometry, such as core-sets, and commutative algebra that is used for solving the polynomial system. While PnP was selected for demonstration, we expect applications to many other open problems, especially in computer vision.

## 4.6 An optimal transport model for dynamical shapes, collective motion and cellular aggregates

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Many living and physical systems such as cell aggregates, tissues or bacterial colonies behave as unconventional systems of particles that are strongly constrained by volume exclusion and shape interactions. Understanding how these constraints lead to macroscopic self-organized structures is a fundamental question in e.g. developmental biology. To this end, various types of computational models have been developed. Here, we introduce a new framework based on optimal transport theory to model particle systems with arbitrary dynamical shapes and deformability properties. Our method builds upon the pioneering work of Brenier on incompressible fluids and its recent applications to materials science. It lets us specify the shapes and volumes of individual cells and supports a wide range of interaction mechanisms, while automatically taking care of the volume exclusion constraint at an affordable numerical cost. We showcase the versatility of this approach by reproducing several classical systems in computational biology. Our Python code is freely available at <https://iceshot.readthedocs.io/en/latest/>

## 4.7 Data-driven stereology: Integrating generative adversarial networks with tessellation-based models for 3D microstructure reconstruction

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Many natural materials exhibit a cellular microstructure, where the material is composed of individual cells or domains with distinct properties, despite sharing the same composition. Such structures are observed, for example, in metallic materials, biological systems, synthetic materials like foams and rocks. The spatial arrangement, size distribution, interfacial characteristics and morphological features of these cells critically determine the macroscopic effective properties of the bulk material. Consequently, the investigation of cellular structures is of great importance. Tessellations provide a natural and mathematically rigorous framework for partitioning space into cells, making them particularly well suited for modeling cellular microstructures. Their parameters have clear geometric interpretations, such as cell size, shape and adjacency, which directly correspond to observable microstructural characteristics.

By combining point stochastic processes with distance-based tessellation models such as Poisson–Voronoi and Laguerre tessellations, it becomes possible to generate random tessellations whose realizations are statistically similar to those observed in experimental image data [1]. This allows the efficient generation of large datasets of model realizations, facilitating the systematic investigation of structure–property relationships. However, 3D datasets, that are usually required for calibrating such random 3D tessellation models are often unavailable due to the high cost or complexity of their acquisition.

This talk addresses this issue, by introducing a data-driven framework that leverages parametric tessellation models to statistically calibrate 3D random tessellation models using only 2D image data while preserving morphological interpretability[2, 3]. Specifically, we

employ generative adversarial networks (GANs) to learn the tessellation parameters from 2D images, enabling efficient inference of realistic 3D cellular morphologies without the need for expensive 3D measurements. This approach bridges the gap between physically interpretable stochastic geometry and the generative capabilities of deep learning. It offers a data-efficient pathway for reconstructing and simulating realistic 3D microstructures, supporting applications in materials design, stereological analysis and computational materials science.

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## 4.8 Geometric properties of random Laguerre tessellations

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Joint work of Anna Gusakova, Mathias in Wolde-Lübke

In this talk we consider stationary random Laguerre tessellations whose generating point set is given by some inhomogeneous Poisson point process in space-time  $\mathbb{R}^d \times \mathbb{R}$ . We will discuss sectional properties of Poisson-Laguerre tessellations revealing their relation to the classical Poisson-Voronoi tessellation. Furthermore, we will study the class of the corresponding dual Laguerre tessellations which, under some natural assumptions, give rise to simplicial random tessellations. For these models we will be interested in the geometric properties of their typical cell.

## 4.9 The Road to the Closest Point is Paved by Good Neighbors

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Joint work of Sariel Har-Peled, Benjamin Raichel, Eliot W. Robson

Main reference Sariel Har-Peled, Benjamin Raichel, Eliot W. Robson: “The Road to the Closest Point is Paved by Good Neighbors”, in Proc. of the 2026 Symposium on Simplicity in Algorithms, SOSA 2026, Vancouver, BC, Canada, January 12-14, 2026, pp. 1–11, SIAM, 2026.

URL <https://doi.org/10.1137/1.9781611978964.1>

Given a set  $P$  of  $n$  points in  $\mathbb{R}^d$ , and a parameter  $\varepsilon \in (0, 1)$ , we present a new construction of a directed graph  $G$ , of size  $O(\frac{n}{\varepsilon^d})$ , such that  $(1 + \varepsilon)$ -ANN queries can be answered by performing a greedy walk on  $G$ , repeatedly moving to a neighbor that is (significantly) better than the current point. To the best of our knowledge, this is the first construction of a linear size with no dependency on the spread of the point set. The resulting query time, is  $O(\varepsilon^{-d} \log \Psi)$ , where  $\Psi$  is the spread of  $P$ . The new construction is surprisingly simple and should be practical.

## 4.10 Stochastic Microstructure Modelling Based on Random Tessellations

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**Joint work of** Christian Jung, Katja Schladitz, Claudia Redenbach

**Main reference** Christian Jung, Claudia Redenbach: “Crack Modeling via Minimum-Weight Surfaces in 3d Voronoi Diagrams”, in *Journal of Mathematics in Industry*, 13(10), 2023.

**URL** <https://doi.org/10.1186/s13362-023-00138-1>

Modelling the microstructure of industrial materials allows for the generation of large synthetic data sets that can be used for numerical simulations and the training of machine learning models. In this talk we consider stochastic microstructure models based on random tessellations and several applications. First, we establish a model for crack structures in concrete. Cracks are assumed to take the path of least resistance when propagating through concrete. The model is based on the idea of weighting the facets of a 3d Voronoi tessellation. Bounded by a contour, a connected set of facets of minimal weight is computed by solving a binary integer program. The point process models that generate the Voronoi diagrams are interchangeable such that the model realizations show several levels of regularity. This makes the model highly flexible and allows for the generation of a whole range of different crack structures. Second, germ-grain processes based on the cells of Gibbs-Laguerre tessellations are used for modelling solid particles in active protective coatings. Our goal is to compute realizations of Gibbs-Laguerre tessellations whose distributions of cell shape and size are similar to those of the observed particles. Several techniques are proposed to also account for the correlation between these characteristics.

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## 4.11 When grains go wild! Tracking the emergence and persistence of abnormal grain growth using time-resolved 3D x-ray microscopy

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**Joint work of** Carl Krill, André Schulz-Harder, Jule M. Dake, Karolína Gutbrod, Madlen Atzen, Markus Ziehmer, Thomas Wilhelm, Orkun Furat, Volker Schmidt, Haixing Fang, Pierre-Olivier Autran, Wolfgang Ludwig

Usually, the coarsening of a polycrystalline material is a rather civilized affair: adjacent grains exchange atoms at moderate rates, only a small fraction of grains disappears over a given interval, and the grain-size distribution remains unimodal. In some systems, however, certain participants in this competition develop a seemingly insatiable appetite for growth! The

resulting microstructure features a subpopulation of oversized, *abnormal* grains embedded in a matrix of much smaller ones, producing the characteristic bimodal grain-size distribution associated with abnormal grain growth (AGG).

Despite the prevalence of AGG, the conditions that trigger the first abnormal grains and the mechanisms that sustain their growth remain poorly understood. To address these questions, we have used time-resolved diffraction-contrast tomography (DCT) to capture the evolution of AGG in three dimensions in the commercial aluminum alloy 5252. These measurements, supplemented by phase-contrast tomography to map second-phase pinning particles, reveal persistent migration of abnormal/matrix interfaces through a dense particle field. However, the *rate* of such migration is observed to be strongly correlated with the number density of particles encountered by each boundary.

Together, the time-resolved observations suggest that a single underlying mechanism may be responsible for both the emergence of abnormal grains and the persistent growth of these grains at the expense of the surrounding matrix.

#### 4.12 Semi-discrete convex order and Laguerre tessellation fitting

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Joint work of David P. Bourne, Thomas O. Gallouët, Quentin Merigot, Andrea Natale

Laguerre tessellations offer a computationally tractable way to describe a large number of convex partitions of Euclidean space. For this reason, they have become popular in computational geometry, imaging and numerical analysis, both as a modeling and a discretization tool.

In material science, Laguerre tessellations are used to describe the microstructure of polycrystals. In this context, one generally needs to fit various type of data describing polycrystalline structures by means of tessellations. Motivated by these applications, we study the problem of recovering the generators and weights associated with a given Laguerre tessellation, provided the volumes and barycenters of its cells, which is an idealized version of a common scenario encountered in practice [3].

To solve this problem, we make explicit the connection between barycenters obtained from Laguerre tessellations with prescribed cell volumes and semi-discrete Optimal Transport [4], developing a point of view proposed in [2]. Specifically, we find that any vector of barycenters arising from a Laguerre tessellation of cells with prescribed volumes can be understood as an exposed point of a convex set  $C$  defined by convex order relations [1]. Moreover, maximizing a linear function over this set is equivalent to solving a semi-discrete Optimal Transport problem. We leverage this characterization to propose a numerical algorithm that approximately solves the reconstruction problem by computing an orthogonal projection onto  $C$ . This can be computed efficiently using classical convex optimization algorithms. Importantly, the proposed approach can be used more generally on experimental data which does not necessarily arise from a Laguerre tessellation, which is the typical scenario in the material science applications motivating this work.

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### 4.13 From classical models to Voronoi diagrams with graph-valued seeds – applications to morphological modeling in materials science

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Stochastic 3D modeling of the morphology of micro- and nanostructures allows for generating large databases that can be used to quantify relationships between morphology and effective physical properties of functional materials, such as polycrystalline materials, fuel cells or porous silica. The latter is crucial for resource-efficient optimal design of these materials. In this talk, we present three different parametric morphological models based on random tessellations. First, we show a parametric model based on marked tessellations developed for polycrystalline materials, which exhibit so-called twinning effects. This requires a particular dependency structure for the  $SO(3)$ -valued marks which model the crystal orientations of the grains [1]. Second, we discuss a model for three-phase structures in solid oxide fuel cell anodes that guarantees that all three phases are almost surely connected. For this purpose, a special kind of Voronoi diagram is used that consists only of three cells, and the seeds are three independent random graphs. The vertices of the latter are modeled by homogeneous Poisson point processes [2, 3]. A generalization of this model leads to the third application, where the morphology of porous silica is modeled. In this case, the vertices of the random graphs are modeled by Matérn cluster processes. The model is then fitted to three differently manufactured samples of porous silica [4]. Finally, an outlook on future research and open problems regarding the considered models are presented.

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#### 4.14 Voronoi-like graphs with applications

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**Main reference** Evanthia Papadopoulou: “Abstract Voronoi-Like Graphs: Extending Delaunay’s Theorem and Applications”, in Proc. of the 39th International Symposium on Computational Geometry, SoCG 2023, Dallas, Texas, USA, June 12–15, 2023, LIPIcs, pp. 52:1–52:16, Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2023.

**URL** <https://doi.org/10.4230/LIPICS.SOCG.2023.52>

Abstract Voronoi diagrams (AVDs) offer a unifying framework for various concrete Voronoi diagrams involving points and generalised sites, such as segments, disks, or polygons, in various metrics. Rather than the geometric notions of sites and circles, AVDs are based on bisecting curves that satisfy some simple combinatorial properties. In this talk I will give an overview of AVDs and define a more relaxed Voronoi-like variant. Voronoi-like diagrams are graphs in the arrangement of bisecting curves that fall under the abstract framework, whose vertices are “locally Voronoi” corresponding to vertices in Voronoi diagrams of three sites. Voronoi-like graphs turn out to be Voronoi diagrams subject to perhaps missing some faces, if Voronoi regions can be disconnected. This result extends Delaunay’s theorem beyond points in the Euclidean plane, to Voronoi diagrams that fall under the AVD framework. We have used Voronoi-like graphs to derive expected linear-time algorithms to compute Voronoi trees and forests. We also expect Voronoi-like graphs to be relevant to Voronoi recognition problems.

#### 4.15 Statistics of random marked tessellations

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**Joint work of** Zbynek Pawlas, Viktor Beneš, Daniela Flimmel, Luděk Heller, Iva Karafiátová, Jesper Møller, Filip Seitzl, Jakub Staněk, Joseph E. Yukich

We present an overview of several statistical problems arising in the analysis of random marked tessellations. First, we consider non-parametric estimation of the grain-mark distribution. Using the minus-sampling technique, we construct an unbiased estimator of Horvitz–Thompson type. For a stationary weighted Voronoi tessellation generated by a Poisson point process, we establish variance asymptotics, weak consistency, and asymptotic normality under mild conditions on the weights of the cells in [1].

The second problem is motivated by applications in materials science and concerns the fitting of parametric models for marks taking values in  $SO(3)$ . Conditional on the Laguerre tessellation, we propose in [2] interaction models for the distribution of cubic crystal lattice orientations, where interactions occur between pairs of orientations associated with neighbouring cells of the tessellation.

Finally, we describe a statistical test introduced in [3] for deciding whether orientations are assigned independently to the cells of the underlying tessellation. The distribution of a given orientation may either be identical for all cells or depend on the corresponding cell. For both settings, non-parametric tests are developed.

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## 4.16 A Historical Perspective on the Use of Generalised Voronoi Diagrams in Polycrystal Mechanics

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In materials science, particularly in polycrystal mechanics, simulation is essential for studying the mechanical response and microstructure evolution of materials under external loads. Because polycrystalline materials have random microstructures, generalized Voronoi tessellations are the preferred approach for representing them. However, the appropriate model must be used for each application, which is why models of different levels of refinement have been used in the past. In the 1990s, simulations focused on replicating macroscopic properties, such as strain-strain response and crystallographic texture – i.e., the statistical distribution of the crystal orientations of the grains. In this context, and to facilitate mesh generation, researchers widely used regularly shaped grains, such as cubes, dodecahedra, and truncated octahedra. As experimental methods became available to probe local deformation or microstructural evolution during straining, simulations matured as well. Voronoi tessellations emerged as dominant polycrystal models. However, Poisson Voronoi tessellations contain a large number of small edges, posing a problem for simulations based on the finite element method. A “regularization” technique was developed to solve this problem and enable robust simulations up to 30–40% strain [1]. The next experimental breakthrough involved three-dimensional (3D) measurements of microstructural and mechanical states during deformation using high-energy X-ray diffraction. Around the same time, Laguerre tessellations were first used as polycrystal models. In an optimization context, Laguerre tessellations can be generated from any form of input, whether statistical, incomplete (e.g., grain centroids and volumes), or complete (e.g., polycrystal map) [2]. Despite the resulting convexity of the grains, which is not necessarily present in a real polycrystal, it was shown that the main properties of an experimental deformation field can be accurately reproduced [3]. The latest X-ray diffraction methods allow the elastic strain field in a deformed polycrystal to be mapped on a per-voxel basis. This again requires new developments in polycrystal modeling. Anisotropic power diagrams can reproduce the non-convexity of grains with remarkable agreement with real microstructures. However, meshing such microstructures remains an open problem. Similarly, microstructures obtained using new processing techniques, such as additive manufacturing, differ significantly from those obtained using traditional techniques, which presents an additional challenge for microstructure modeling.

Neper is an open-source software package designed for polycrystal modeling based on generalized Voronoi tessellations, especially for comparative studies between experiments and finite element simulations [4]. When used with its companion program, FEPX, Neper

provides a complete workflow, from tessellation generation to managing, processing, and visualizing simulation results [5]. As Neper is a large open-source program, it is a potential platform for efficiently implementing new methods.

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## 4.17 Statistical Inference for Poisson-Laguerre tessellation: inversion and reconstruction

Martina Vittorietti (TU Delft, NL)

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**Main reference** Thomas van der Jagt, Geurt Jongbloed, Martina Vittorietti: “Nonparametric inference for Poisson-Laguerre tessellations”, Scandinavian Journal of Statistics, Vol. 52(4), pp. 1816–1851, 2025.  
**URL** <https://doi.org/10.1111/sjos.70011>

In this talk, we consider statistical inference for Poisson-Laguerre tessellations in  $\mathbb{R}^d$ . The object of interest is a distribution function  $F$  which describes the distribution of the arrival times of the generator points. The function  $F$  uniquely determines the intensity measure of the underlying Poisson process. We consider two scenarios: first, we assume to know the points of the Poisson process which generate non-empty cells and the actual cells corresponding to these points and construct two nonparametric estimators. The proposed estimators are proven to be strongly consistent, as the observation window expands unboundedly to the whole space. Then, we assume to do not know the points and to want to retrieve them inverting the tessellation. We provide sufficient conditions for consistently inverting the observed Poisson-Laguerre tessellation, as the observation window expands unboundedly to the whole space. The performance of the two estimators, previously proposed is investigated also in this setting.

## 5 Working Groups

In the working group sessions, the participants split up into smaller groups. The discussions mainly evolved around two topics: algorithmic problems related to generalized Voronoi diagrams and the use of generalized Voronoi diagrams in materials science applications. The composition of the groups differed from session to session.

## 5.1 Algorithms and Data Structures

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### Discussed Problems

This group discussed methods for reconstructing Laguerre tessellations from incomplete data, such as the volumes and centroids of the cells. We compared various methods from different communities including stochastic optimisation (the cross-entropy method), stochastic geometry, and optimal transport theory.

Another topic of the discussion was the lack of efficient data structures for storing diagrams with curved cell boundaries such as generalized balanced power diagrams. We also discussed efficient algorithms for computing such diagrams.

## 5.2 Materials Applications

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### Discussed Problems

The groups discussed various aspects related to the modelling of materials microstructures. A particular focus was on representing the grain system in polycrystalline materials.

In many applications, only fitting of the grain size distribution is considered. Grain sizes are often observed empirically to follow approximately log-normal distributions, although this behavior is not universal and its theoretical justification remains largely phenomenological. For realistic grain systems, also grain shape including anisotropy should be taken into account. In particular, large cells of Laguerre diagrams often turn out to be too spherical when compared to real grains.

For finite element simulations, the cells of the diagram have to be meshed. Short cell edges can result in computationally inefficient meshes. Hence, a regularization step that resolves short edges should be applied prior to the mesh generation.

Differences between the microstructure of additively manufactured materials and materials produced by conventional approaches were discussed. While additive manufacturing gives more control on the large scale structure, it results in very chaotic microstructures that pose new challenges for microstructure modelling. This is a particular problem for parts with complex shapes which induce massive edge effects that must be reproduced in the model. Simply masking a homogeneous tessellation model with the desired shape is not a solution to this problem.

The observation and modelling of grain growth in polycrystalline materials was another topic of a lively discussion. In particular, individual grains disappear during grain growth. The resulting topological changes in the diagram must be correctly reproduced. This, in turn, underscores the importance of analytic boundary representations for materials science applications, since they enable the inference of geometric properties such as dihedral angles.

It was further suggested that, rather than first inferring geometric quantities such as volumes and centres of mass from diffraction data and subsequently constructing a generalized Voronoi diagram, it may be possible to reconstruct such diagrams directly from diffraction data using learning-based methods, potentially reducing modelling bias and improving computational efficiency.

## 6 Software Demos

### 6.1 Neper (Romain Quey)

Romain Quey gave a demonstration of how to use the software for polycrystal generation and how to visualize and output its results.

“Neper is a free / open source software package for polycrystal generation and meshing. It can be used to generate polycrystals with a wide variety of morphological properties, from very simple morphologies (simple tessellations, grain-growth microstructures, ...) to complex, multiphase or multiscale microstructures that involve grain subdivisions. The resulting tessellations can be meshed into high-quality meshes suitable for finite-element simulations.” (Source: <https://neper.info/>).

### 6.2 SynthetMic (David Bourne)

David Bourne gave a demonstration of his software library *SynthetMic* (<https://github.com/synthetic-microstructures/synthetmic>), which was developed in collaboration with R. O. Ibraheem (M-DICE, Heriot-Watt University) and S. M. Roper (University of Glasgow). This is a python library for generating 2D and 3D synthetic polycrystalline microstructures using Laguerre tessellations. It includes a fast algorithm for generating grains of prescribed volumes using optimal transport theory. The demo focused on the graphical user interface (web app) for the library, which can be found here: <https://david-bourne.shinyapps.io/synthetmic-gui/>.

### 6.3 Geogram (Bruno Lévy)

Bruno Lévy gave a demonstration of his geometry-processing library *Geogram* (<https://github.com/BrunoLevy/geogram>) and a tutorial on how to install it. Geogram includes code for meshing, Delaunay triangulations, Laguerre diagrams, and solving semi-discrete optimal transport problems.

## Participants

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