

# Comparative Analysis of Algorithms for the Fitting of Tessellations to 3D Image Data

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## Abstract

This paper presents a comparative analysis of algorithmic strategies for fitting tessellation models to 3D image data of materials such as polycrystals and foams. In this steadily advancing field, we review and assess optimization-based methods—including linear and nonlinear programming, stochastic optimization via the cross-entropy method, and gradient descent—for generating Voronoi, Laguerre, and generalized balanced power diagrams (GBPDs) that approximate voxel-based grain structures. The quality of fit is evaluated on real-world datasets using discrepancy measures that quantify differences in grain volume, surface area, and topology. Our results highlight trade-offs between model complexity, the complexity of the optimization routines involved, and the quality of approximation, providing guidance for selecting appropriate methods based on data characteristics and application needs.

**Keywords:** Tessellation, Voronoi diagram; Laguerre diagram; generalized balanced power diagram; linear programming; non-linear programming; gradient descent; cross-entropy method; polycrystal; foam

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# 1 Introduction

The past two decades have witnessed the emergence and rapid growth of 3D materials science, driven by progress in both experimental instrumentation and computational modeling; see, e.g., [1, 2, 3]. For polycrystalline materials, a central aim is to correlate experimentally measured 3D grain maps with three-dimensional simulations, particularly in the study of phase transformations, plasticity, and grain growth. These developments have enabled unprecedented insights into the microstructural evolution of polycrystalline materials (see, e.g., [4, 5, 6, 7, 8]) and have catalyzed the creation of modeling frameworks that balance geometric fidelity and computational cost (see, e.g., [9, 10, 11, 12, 13]).

Similarly to the grains in polycrystalline materials, the cells in foams also form a space-filling system of almost polyhedral cells. Therefore, both material classes can be described with similar mathematical models. The cell structure of foams can be imaged in 3D using micro-computed tomography ( $\mu$ CT). Stochastic models fitted to the image data then allow for a systematic investigation of properties such as elasticity, permeability, or heat conduction [14, 15, 16].

In this paper, we consider 3D image data from polycrystalline materials as well as from three distinct types of foams, with tessellation models analyzed for both material classes. To keep the wording concise, we will use the term *grain* both for the grains in polycrystalline materials and the cells in a foam. The term *cell* will refer to the tessellation cells in the fitted models.

## 1.1 Tessellation models

Tessellation models play a central role in 3D materials science. By representing the grain structure as a spatial partitioning of the domain into cells, often convex, but potentially non-convex, these models can offer a compact and analytically tractable approximation of the grain network. A sparse representation, depending on a small number of parameters, is especially advantageous for simulations: grain boundary geometries can be stored efficiently, and their analytic descriptions allow for fast and accurate computation of geometric and topological quantities in downstream tasks. Moreover, fitting tessellations can suppress high-frequency noise in experimental data, enabling more robust geometrical and statistical analyses. They also facilitate the study of morphological features such as grain size distributions, anisotropy, and neighborhood statistics, which are critical to understanding material behavior under mechanical and thermal loads.

Among the various tessellation models, *power diagrams*—also known as *Laguerre* or *Voronoi-Laguerre diagrams* [17, 18]—and their generalizations, *generalized balanced power diagrams* (also known as *anisotropic power diagrams*) [11, 19] have emerged as particularly versatile tools. These structures have found diverse applications, extending beyond microstructure modeling and grain growth simulations [20, 21, 22] to include imaging [23], spatial statistics [24, 25], mesh generation [26, 27], and machine learning [28]. For detailed reviews of these applications, see, for example, [29, 30, 31, 32] and the review articles [18, 33, 34].

In this paper, we investigate several algorithmic approaches for fitting tessellation models, namely Voronoi, Laguerre, and generalized balanced power diagrams (GBPDs) to volumetric image data of materials such as polycrystals and foams. We explore a range of optimization techniques, from linear programming methods to stochastic and gradient-based algorithms, evaluating their effectiveness in capturing complex microstructural geometries. Through comparative experiments on real datasets, we highlight the trade-offs between the complexity of the optimization methods and the accuracy of the resulting tessellation approximations, aiming to guide the selection of suitable approaches for various application scenarios.

## 1.2 Fitting or approximation

Modeling the 3D morphology of polycrystals or foams requires finding suitable model classes which can accurately represent the grain systems observed in data. This task can be interpreted in several ways.

*Fitting or approximation*, the focus of this paper, refers to the task of finding a set of generators in a given model class, e.g., a Laguerre tessellation, such that the tessellation induced by the generators

gives a good fit to the observed grain system. The goodness of fit is measured by suitable discrepancy measures. We do not make the restrictive assumption that the material must fit exactly within one of the model classes, i.e., that the approximation error must be zero. When this assumption is enforced, the task is referred to as *inversion* in the literature [35, 36, 37]. The goal of both fitting and inversion is to generate highly accurate representations that can be directly used in downstream applications, such as automated analysis, simulation, or visualization.

Fitting and inversion approaches have been suggested for several types of data, i.e., for different representations of grain systems. The grain systems/tessellations might be represented as a collection of subsets of the Euclidean space, or analytic boundary descriptions might be given. Examples of approaches that work directly with such data are given in [35, 37, 38]. The problem of approximating an arbitrary input tessellation with a Voronoi tessellation is addressed in [35], and extended in [38] to the more general case of Laguerre tessellations. The central objective is to minimize the total mismatch volume between the grains/cells of the observed grain systems and the approximating tessellations, which is achieved via a gradient descent-based optimization method. The problem of inverting a Laguerre tessellation was solved in [37].

### 1.3 Optimization methods

If the grain system to be modeled is observed as voxel data, typically, modeling approaches voxelize tessellation cells as well. In [11], the authors present a fitting technique by solving a linear program. It uses the relation of tessellations and optimal clusterings and formulates the problem of fitting the tessellations as a weight-balanced least-squares assignment problem. In [39], a non-linear optimization method is introduced that minimizes the distances between the observed grain system and the tessellation. As an alternative, stochastic optimization methods such as simulated annealing [40] and a cross-entropy method [41, 42] were proposed. In these approaches, the generators of the tessellation are iteratively modified. Then, updated generators are accepted with a probability based on the quality of the current fit.

Some experimental techniques, such as X-ray diffraction microscopy [2], do not directly measure all grain parameters; instead, some or all of them are indirectly inferred from the measurements. For example, only volumes and centers of mass are reported in [10, 11, 43]. In this case, Lyckegard et al. [10] propose a simple heuristic to choose the generators of an approximating Laguerre tessellation. This heuristic is often chosen as initial configuration for optimization methods which then further improve the fit to real data. The approach of [11] can also deal with such indirect data; additionally, volume limits can be incorporated into the fit.

Approaches can also vary in terms of the tessellation types they generate. Voronoi and Laguerre tessellations as generated by [35] and [10, 37, 38], respectively, assume that the observed structure is isotropic. However, this assumption does not always hold and individual grains can indeed exhibit strong anisotropy [19]. In such cases, tessellations with elliptical generators such as GBPDs are superior to Laguerre tessellations [44], but require higher computational effort when fitting them to data. Some of the optimization techniques discussed above, e.g., the linear programming approaches [11, 45], simulated annealing [40] or gradient descent-based methods [43], can also be applied to GBPDs. In the present paper, we review various algorithms for approximating the data with tessellation models of increasing complexity. Therefore, we deploy different combinations of fitting algorithms and tessellation models to several voxelized datasets, followed by an extensive quantitative comparison. Table 1 summarizes the algorithms considered along with their respective inputs and outputs. The diagram types underlying these algorithms are introduced in Section 2, while the fitting algorithms are detailed in Section 3.

### 1.4 Stochastic reconstruction methods

In contrast to the approximation methods considered here, *parametric* and *nonparametric stochastic reconstruction* methods are designed to generate microstructures that match statistical features rather than exact geometry, making them effective for synthetic data generation [15, 16]. In parametric stochastic modeling, the parameters of a specific model, e.g. of a homogeneous Poisson-Voronoi tessellation,

have to be determined such that the model realizations exhibit cells that reproduce statistics of the observed grains, e.g., the grain size distribution, see [46, 47]. In stochastic reconstruction, a stochastic, nonparametric optimization approach is used to construct a random tessellation fitting certain predefined statistics, see [39, 48].

	Input Data		Output Diagram			
	voxelized	indirect	Voronoi	Laguerre	d-GBPD	GBPD
H <sub>0</sub>	✓	✓	✓	✓	✓	✓
H <sub>q</sub>	✓	✓	–	✓	✓	✓
LP	✓	✓	–	✓	✓	✓
CE	✓	–	–	✓	–	–
GD I	✓	–	✓	✓	✓	✓
GD II (Neper)	✓	✓	✓	✓	–	–

Table 1: Comparison of the fitting methods based on direct input data (discretized grains) and indirect input data (grain volumes and barycenters), as well as with respect to their output data. The symbol ‘✓’ in the output columns indicates that the respective diagram type can be specified and guaranteed as output.

## 2 Tessellation models

Tessellations can generally be defined in an arbitrary dimension  $d \geq 1$ . We restrict our attention to the case  $d = 3$ . Let  $\phi \subseteq \mathbb{R}^3$  be a non-empty locally finite set of sites in  $\mathbb{R}^3$ , where locally finite means that any bounded subset of  $\mathbb{R}^3$  only contains a finite number of elements of  $\phi$ . The points  $x \in \phi$  are called generators. For our application, it is sufficient to consider finite sets of generator points such that the sites are contained in a bounded observation window  $V \subset \mathbb{R}^3$ .

The *Voronoi tessellation* of  $\phi$  is the collection of all cells of the form

$$C(x, \phi) = \{y \in \mathbb{R}^3 : \|y - x\| \leq \|y - x'\| \text{ for all } x' \in \phi\}, \quad (1)$$

for each  $x \in \phi$ , with  $\|\cdot\|$  denoting the Euclidean norm in  $\mathbb{R}^3$ .

Generalizations of the Voronoi tessellation are obtained by assigning real-valued weights  $w$  to the generators  $x$  which are then incorporated into the distance measure. Let now  $\phi \subseteq \mathbb{R}^3 \times \mathbb{R}$  be a locally finite set of weighted generators. Then, the *Laguerre tessellation* of  $\phi$  is the collection of all non-empty cells of the form

$$C((x, w), \phi) = \{y \in \mathbb{R}^3 : \|y - x\|^2 - w \leq \|y - x'\|^2 - w' \text{ for all } (x', w') \in \phi\}, \quad (2)$$

for each  $(x, w) \in \phi$ . If all weights are equal, the special case of a *Voronoi tessellation* is obtained. Laguerre tessellations are also known as *power diagrams* or *additively weighted Voronoi diagrams*.

The ‘distance’  $\text{pow}((x, w), y) = \|y - x\|^2 - w$  is called the *power* of  $y$  with respect to  $(x, w)$ . In addition, the definition  $\text{pow}((x, w), y) = \|y - x\|^2 - w^2$  can also be found in the literature. In this case, a generator  $(x, w)$  can be interpreted as a ball with center  $x \in \mathbb{R}^3$  and radius  $r = |w| \geq 0$ . For points  $y$  outside this ball, the power distance  $\text{pow}((x, w), y)$  measures the squared length of the tangent line from  $y$  to the ball.

A further generalization can be obtained by assigning to each generator a symmetric positive definite matrix. We again retain the notation  $\phi$  for this extended set of generators, with elements denoted by  $(x, M, w)$ , where  $M$  is a symmetric positive definite  $3 \times 3$  matrix. Given such an extended set  $\phi$  of generators, the cells of the *generalized balanced power diagram* (GBPD) are defined as

$$C(\mathbf{x}, \phi) = \{y \in \mathbb{R}^3 : (y - x)^\top M(y - x) - w \leq (y - x')^\top M'(y - x') - w' \text{ for all } (x', M', w') \in \phi\}, \quad (3)$$



for each  $\mathbf{x} = (x, M, w) \in \phi$ . Special cases of GBPDs are obtained, for example, by only considering diagonal positive definite matrices (d-GBPD) or by setting all weights  $w$  to 0. In the literature, GBPDs are also referred to as *anisotropic power diagrams*.

Examples of planar tessellation models ( $d = 2$ ) and their generators are shown in Figure 1, where the generator sets are drawn from a homogeneous Poisson point process in the unit square  $[0, 1]^2$ , without marks and with appropriately chosen (independently sampled) marks. More information on tessellation models can be found, e.g. in [29, 30, 49].

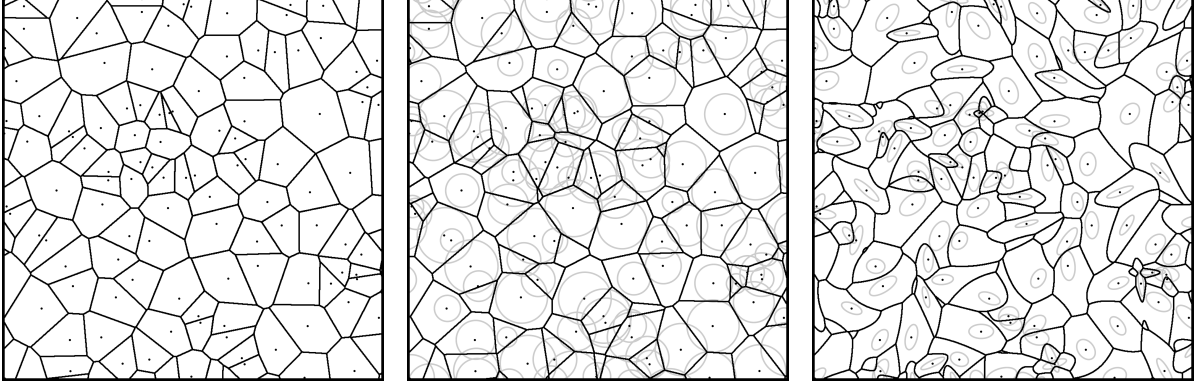


Figure 1: Examples of planar tessellations drawn from a Poisson point process of intensity  $\lambda_{Poi} = 100$  in the unit square: A Voronoi tessellation (left), a Laguerre tessellation (middle) with independently sampled weights  $w$  (visualized by the radii of the corresponding discs) uniformly distributed on the interval  $[0.025, 0.075]$ , and a GBPD with independently sampled  $2 \times 2$  matrices  $M$  representing ellipses with semi-major axes lengths uniformly distributed on  $[0.024, 0.042]$ , semi-minor axes lengths on  $[0.006, 0.024]$  and uniform rotations on  $[0, \pi]$ .

### 3 Algorithms

The input for all algorithms is a discretized grain structure given on a grid of voxel coordinates  $W = V \cap \mathbb{Z}^3$  for some set  $V \subset \mathbb{R}^3$ , where  $\mathbb{Z} = \{\dots, -1, 0, 1, \dots\}$ . Throughout this paper, we will denote the number of elements in  $W$  by  $m \in \mathbb{N} = \{1, 2, \dots\}$ . In particular, a discretized structure on  $W$  comprising  $n \in \mathbb{N}$  grains is represented by a mapping

$$\text{GT} : W \rightarrow \{0, \dots, n\}, \quad (4)$$

which is also referred to as *grain scan* or *grain map*. The  $i$ th grain of GT is then defined by  $C_i^{\text{GT}} = \{x \in W : \text{GT}(x) = i\}$ . We assume that the cardinality  $|C_i^{\text{GT}}|$  of  $C_i^{\text{GT}}$  fulfills  $|C_i^{\text{GT}}| > 1$  for each  $i \in \{1, \dots, n\}$ . Typically,  $\{x \in W : \text{GT}(x) = 0\}$  is not a grain, but is either the empty set or the set of voxels that separate neighboring grains.

To fit a Voronoi (or Laguerre) tessellation to a mapping GT as given in (4), we consider the set of all Voronoi (or Laguerre) tessellations of  $V$  that are induced by  $n$  generators. In the Laguerre case, each element of this set can be represented by a (not necessarily unique) set  $\phi = \{(x_1, w_1), \dots, (x_n, w_n)\} \subseteq \mathbb{R}^3 \times \mathbb{R}$  of  $n$  generators. For each  $i \in \{1, \dots, n\}$ , it defines a cell  $C_i(\phi) = C((x_i, w_i), \phi)$  as given by Eq. (2). The Voronoi case is then obtained by setting  $w_i = 0$  for each  $i \in \{1, \dots, n\}$ . For GBPDs, we use an analogous procedure where the generator sets are of the form  $\phi = \{(x_1, M_1, w_1), \dots, (x_n, M_n, w_n)\}$  and  $C((x_i, M_i, w_i), \phi)$  is given by Eq. (3), for each  $i \in \{1, \dots, n\}$ . For Voronoi and Laguerre tessellations as well as GBPDs, the set of all tessellations in  $V$  generated by exactly  $n$  generators will be denoted by  $\Phi_n$ . Note that in the case of Laguerre tessellations and GBPDs, the tessellations in  $\Phi_n$  can have fewer than  $n$  cells.

### 3.1 Heuristics

Two heuristics have been introduced in the literature that avoid optimization routines, as the generators for Voronoi and Laguerre tessellations and GBPDs are directly estimated from the data. The heuristics, henceforth referred to as  $H_0$  [19] and  $H_q$  [10, 50], differ in their setting of the weights  $w_i$ ,  $1 \leq i \leq n$ . In  $H_0$ , all weights  $w_i$  are set to zero which leads to a Voronoi tessellation. In contrast, under  $H_q$ , the weights are defined as

$$w_i = \left( \frac{3|C_i^{GT}|}{4\pi\sqrt{\det(B_i)}} \right)^{2/3}, \quad i \in \{1, \dots, n\},$$

where the matrices  $B_1, \dots, B_n$  depend on the specific model. In the Laguerre case,  $B_1, \dots, B_n$  are taken to be the identity matrix, as in [10]. In the GBPD case [50],  $B_i$  is set to the sample covariance matrix of the region  $C_i^{GT}$ , given by

$$B_i = \Sigma(C_i^{GT}) = \frac{1}{|C_i^{GT}| - 1} \sum_{y \in C_i^{GT}} (y - c(C_i^{GT}))(y - c(C_i^{GT}))^\top, \quad i \in \{1, \dots, n\}, \quad (5)$$

where  $c(C_i^{GT})$  denotes the barycenter of  $C_i^{GT}$ .

Both heuristics,  $H_0$  and  $H_q$ , have in common that the sites  $x_i$  are set as  $x_i = c(C_i^{GT})$ , and, in the case of GBPDs, the matrices  $M_i$  are derived from a principal component analysis (PCA), where the sample points are all  $y \in C_i^{GT}$ , for each  $i \in \{1, \dots, n\}$ . To be precise,  $M_i$  is given as  $M_i = U_i \Lambda_i^{-1} U_i^\top$  with  $U_i$  denoting the  $3 \times 3$  matrix whose  $j$ th column is the  $j$ th principal component of  $C_i^{GT}$ , for  $j \in \{1, 2, 3\}$ . The corresponding eigenvalues  $\lambda_{i1}, \lambda_{i2}, \lambda_{i3}$  are collected in the diagonal matrix  $\Lambda_i = \text{diag}(\lambda_{i1}, \lambda_{i2}, \lambda_{i3})$  for each  $i \in \{1, \dots, n\}$ , see [50].

An interpretation of the heuristics within the framework of Bayesian classifiers has been given in [22].

### 3.2 Linear programming based approaches [LP]

The linear programming approach introduced in [11], henceforth called LP, computes a GBPD or Laguerre diagram fitting to an observed grain structure, with each of the cells' volumes lying within prescribed bounds  $\kappa_1^-, \dots, \kappa_n^-$  and  $\kappa_1^+, \dots, \kappa_n^+$ . The bounds can either be user-defined and strictly enforced, or uniformly relaxed by assigning  $\kappa_i^- = 0$  and  $\kappa_i^+ = \infty$  for all  $i = 1, \dots, n$ . GBPDs or Laguerre diagrams are generated, depending on the specification or computation of the matrices defining the ellipsoidal norms. Moreover, the approach is flexible in its input requirements, accommodating both indirect data (grain volumes and barycenters), as well as direct input  $C_i^{GT}$ ,  $1 \leq i \leq n$ . Here, we only consider the latter case.

The sites  $x_1, \dots, x_n \in \mathbb{R}^3$  are chosen as the barycenters of the cells. The symmetric positive definite matrices  $M_1, \dots, M_n \in \mathbb{R}^{3 \times 3}$  are computed via a principal component analysis; more precisely,  $M_i$  is set to equal the inverse of the spatial covariance matrix of the set of voxels for grain  $C_i^{GT}$ ,  $1 \leq i \leq n$ ; see also Section 3.1 above. The weights  $w_1, \dots, w_n \in \mathbb{R}$  defining the GBPD are finally obtained from the solution of the dual of the linear optimization problem

$$\begin{aligned} \text{(LP)} \quad & \min \sum_{i=1}^n \sum_{j=1}^m \gamma_{i,j} \xi_{i,j} \\ \text{subject to} \quad & \sum_{i=1}^n \xi_{i,j} = 1 \quad (1 \leq j \leq m), \\ & \kappa_i^- \leq \sum_{j=1}^m \xi_{i,j} \leq \kappa_i^+ \quad (1 \leq i \leq n), \\ & \xi_{i,j} \geq 0 \quad (1 \leq i \leq n; 1 \leq j \leq m), \end{aligned}$$

where  $\gamma_{i,j} = (y_j - x_i)^\top M_i (y_j - x_i)$  and  $y_j$  denotes the position of voxel  $j$  for all  $i \in \{1, \dots, n\}, j \in \{1, \dots, m\}$ . The  $\xi_{i,j}$  are the variables; they specify the fraction of voxels  $y_j$  that are assigned to site  $x_i$ . In the optimum, it can be ensured that these fractions are, in fact, binary due to the special structure of the linear program.

For the results presented in this paper we used the common choice of setting the volume bounds to  $\kappa_i^- = \kappa_i - \varepsilon$  and  $\kappa_i^+ = \kappa_i + \varepsilon$  with  $\varepsilon = 2$  and  $\kappa_i$  denoting the volume of grain  $C_i^{GT}$ . No initial solution is required.

The above LP approach, through its dual formulation, optimizes only the weights  $w_1, \dots, w_n$ . In contrast, the following method from [45], framed within a support vector machine context, optimizes all parameters—that is,  $x_1, \dots, x_n$ ,  $M_1, \dots, M_n$ , and  $w_1, \dots, w_n$ —by solving a linear program. (As before, the weights can be obtained via the dual formulation.) However, this approach does not incorporate volume bounds. Using the notation

$$y_j = \begin{pmatrix} (y_j)_1 \\ (y_j)_2 \\ (y_j)_3 \end{pmatrix}, \quad M_i = \begin{pmatrix} (M_i)_{1,1} & (M_i)_{1,2} & (M_i)_{1,3} \\ (M_i)_{1,2} & (M_i)_{2,2} & (M_i)_{2,3} \\ (M_i)_{1,3} & (M_i)_{2,3} & (M_i)_{3,3} \end{pmatrix},$$

and setting  $a_i = -2M_i x_i$  and  $\alpha_i = x_i^\top M_i x_i + w_i$ , all parameters are encoded in the extended parameter vector  $\mathfrak{M}_i = (\alpha_i, a_i^\top, (M_i)_{1,1}, 2(M_i)_{1,2}, 2(M_i)_{1,3}, (M_i)_{2,2}, 2(M_i)_{2,3}, (M_i)_{3,3})^\top \in \mathbb{R}^{10}$  which yields the variables of the linear program. Setting

$$\mathfrak{Y}_j = (1, (y_j)_1, (y_j)_2, (y_j)_3, (y_j)_1^2, (y_j)_1(y_j)_2, (y_j)_1(y_j)_3, (y_j)_2^2, (y_j)_2(y_j)_3, (y_j)_3^2)^\top,$$

the linear program is then given by

$$\begin{aligned} \min_{(\zeta_j)} \quad & \sum_{j=1}^n \zeta_j \\ \mathfrak{M}_i^\top \mathfrak{Y}_j - \mathfrak{M}_\ell^\top \mathfrak{Y}_j + 1 \quad & \leq 0 \quad (j \in [m], i, \ell \in [n], \ell \neq i, y_j \in \text{int}_{\delta_i}(C_i)), \\ \mathfrak{M}_i^\top \mathfrak{Y}_j - \mathfrak{M}_\ell^\top \mathfrak{Y}_j - \zeta_j \quad & \leq 0 \quad (j \in [m], i, \ell \in [n], \ell \neq i, y_j \in C_i \setminus \text{int}_{\delta_i}(C_i)), \\ \zeta_j \quad & \geq 0 \quad (j \in [m], y_j \in C_i \setminus \text{int}_{\delta_i}(C_i)), \end{aligned}$$

where  $\text{int}_{\delta_i}(C_i) = \{x \in C_i : \|x - x'\| \geq \delta_i \text{ for all } x' \notin C_i\}$  is the  $\delta_i$ -interior of  $C_i$  for user-specified parameters  $\delta_i$ ,  $1 \leq i \leq n$ .

To accelerate computations and reduce memory usage, the calculations for both approaches may be restricted to voxel subsets forming a so-called *coreset*, as described in [45]. Following the procedure in [45], we sample every  $10^{\text{th}}$  voxel along the  $x$ -,  $y$ -, and  $z$ -directions within each input cell, excluding the  $\delta_i$ -interior regions of the cells, with  $\delta_1 = \dots = \delta_n = 20$ .

It should be noted that, in contrast to the other fitting methods discussed in this paper, LP generates a GBPD that adheres to user-specified volume constraints. Remarkably, however, it does not explicitly minimize a discrepancy with respect to the ground truth structure GT within its objective function. The fit appears to reflect the model's capacity to approximate physical processes, for example, those that govern the formation of polycrystalline structures.

### 3.3 Fitting with the cross-entropy method [CE]

In this section, we summarize the method introduced in [41] for fitting Laguerre tessellations to grain structures  $\{C_i^{\text{GT}} : 1 \leq i \leq n\}$  in polycrystalline materials by minimizing an interface-based discrepancy measure, using the cross-entropy method [51], henceforth called CE. For this purpose, we assume that  $V \subset \mathbb{R}^3$  is connected. For any  $i, j \in \{1, \dots, n\}$  with  $i \neq j$ , the discrete interface between two grains  $C_i^{\text{GT}}$  and  $C_j^{\text{GT}}$  is defined by

$$N_{i,j}^{\text{GT}} = \{x \in W : \mathcal{N}_{26}(x) \cap C_i^{\text{GT}} \neq \emptyset \text{ and } \mathcal{N}_{26}(x) \cap C_j^{\text{GT}} \neq \emptyset\},$$

where  $\mathcal{N}_{26}(x)$  denotes the 26-neighborhood of  $x$  in  $W$ , consisting of all voxels that share a face, edge, or vertex with  $x$ ; see Section 3.3 in [52]. Note that  $N_{i,j}^{\text{GT}} = \emptyset$  if and only if  $C_i^{\text{GT}}$  and  $C_j^{\text{GT}}$  are not adjacent. This definition of adjacency means that two grains are also adjacent if they are separated by a line that is one voxel thick. This is a reasonable definition for the original data in [41], where all grains are separated by boundaries that have a thickness of one voxel. Even for data without such separating voxels, the definition of  $N_{i,j}^{\text{GT}}$  is unproblematic since grains that are only one voxel thick do usually not appear in applications.

Based on this notion of neighborhood voxels, we introduce the interface-based discrepancy measure  $E : \Phi_n \rightarrow [0, \infty)$  by

$$E(\phi) = \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{x \in N_{i,j}^{\text{GT}}} \min\{\|x - y\|^2 : y \in C_i(\phi) \cap C_j(\phi)\}. \quad (6)$$

The discrepancy measure  $E$  given in Eq. (6) quantifies the distance between the discretized grain boundaries of the input data and the cell boundaries of the tessellation of  $\phi$ . Minimizing the value of  $E(\phi)$  constitutes a high-dimensional optimization problem, typically characterized by numerous local minima, and the evaluation of the discrepancy measure  $E$  is computationally expensive. Thus, it is proposed in [41] to use the cross-entropy method to minimize an approximation of  $E$ , where—instead of considering all points  $x \in N_{i,j}^{\text{GT}}$ —only a smaller set of test points  $x \in T_{i,j} \subset N_{i,j}^{\text{GT}}$  is considered for any  $i, j \in \{1, \dots, n\}$  with  $i < j$ , see Section 3.4 of [41].

Note that the cross-entropy method [53] is a stochastic optimization method that can be used for parameter fitting. In our case, the parameter vector consists of all generators of the Laguerre tessellation. For a predefined initial parameter vector, the discrepancy measure  $E$  is evaluated for a random sample of 4,000 parameter vectors. Those are assumed to be normally distributed around the initial parameter vector with some variance. Then, the elite set, that is, those 200 parameter vectors for which  $E$  takes the smallest values, is selected. The parameter vector and variance are then updated to equal the mean and variance, respectively, of the parameter vectors in the elite set. This procedure is iterated until the cost function does not decrease significantly for a given number of steps. As an initial parameter vector for the cross-entropy method, the generators obtained from the heuristic Hq are used; see Section 3.1. The authors of [41] made the code for this fitting approach publicly available [54].

In principle, the interface-based discrepancy measure considered in [41] can also be used to fit GBPDs. However, in this scenario, the computation of the minimum distance to the boundary  $C_i(\phi) \cap C_j(\phi)$  is significantly more challenging, rendering the method computationally demanding. Note that in the case of Laguerre tessellations,  $C_i(\phi) \cap C_j(\phi)$  is contained in an affine subspace, such that the analytical determination of the minimum distance given in Eq. (6) can be carried out efficiently.

### 3.4 Gradient descent-based fitting I [GD]

We now consider an algorithm which is based on gradient descent methods, henceforth called GD. For this, in [43], the goodness of fit between the discretized grain structure GT and a GPBD with generator  $\phi$  is measured using the volume-based measure  $E : \Phi_n \rightarrow \mathbb{R}$  given by

$$E(\phi) = \frac{1}{|W|} \sum_{x \in W} \sum_{i=1}^n \lambda\left(\mathbb{1}_{C_i^{\text{GT}}}(x), \mathbb{1}_{C_i(\phi)}(x)\right), \quad (7)$$

where  $\lambda(y, y') \in \mathbb{R}$  measures the similarity between pairs of values  $y, y' \in [0, 1]$ , and  $\mathbb{1}_A$  denotes the indicator of the set  $A \subseteq W$ , defined by  $\mathbb{1}_A(x) = 1$  if  $x \in A$ , and  $\mathbb{1}_A(x) = 0$  if  $x \in W \setminus A$ .

Note that even if  $\lambda$  is differentiable in the second argument, the function  $E$  given in (7) is not differentiable with respect to the GPBD generators  $\phi$ . Hence, maximization of  $E$  based on gradient descent methods is not viable. This problem can be solved by approximating  $E$  with a differentiable objective function. For this purpose, the so-called one-hot encoding was employed in [43].

First, let  $D : W \times \Phi_n \rightarrow \mathbb{R}^n$  be given by  $D(x, \phi) = ((x - x_i)^\top M_i(x - x_i) - w_i)_{i=1}^n$ , i.e., the  $i$ -th component of the vector  $D(x, \phi)$  is the ‘distance’ of  $x$  to the generator point  $\mathbf{x}_i = (x_i, M_i, w_i)$ , for each  $i \in \{1, \dots, n\}$ . Since  $x \in C_i(\phi)$  holds whenever the ‘distance’ from  $x$  to  $\mathbf{x}_i$  is less than or equal to the distance to any other generator point, the second argument of  $\lambda$  in (7) can alternatively be written as

$$\mathbb{1}_{C_i(\phi)}(x) = \text{argmin}_i^*(D(x, \phi)), \quad (8)$$

where  $\text{argmin}_i^*$  denotes the  $i$ -th component of the function  $\text{argmin}^* : \mathbb{R}^n \rightarrow \{0, 1\}^n$ , which maps a vector

$z = (z_1, \dots, z_n) \in \mathbb{R}^n$  to a binary vector indicating the locations of its minimal components. Specifically,

$$\text{argmin}_i^*(z) = \begin{cases} 1, & \text{if } z_i = \min\{z_1, \dots, z_n\}, \\ 0, & \text{otherwise,} \end{cases}$$

for each  $i \in \{1, \dots, n\}$ . That is,  $\text{argmin}_i^*(z)$  is the one-hot (or multi-hot, in case of ties) encoding of the set of indices at which the minimum of  $z$  is attained. Note that  $\text{argmin}_i^*$  is not differentiable everywhere, which transfers also to Eq. (8) and consequently to Eq. (7). To address this issue, in [43], a procedure is proposed to approximate the vector-valued  $\text{argmin}$  function by the softmax function with negated inputs,  $\text{softmax}^*: \mathbb{R}^n \rightarrow [0, 1]^n$ , whose  $i$ -th component is defined as

$$\text{softmax}_i^*(z) = \frac{\exp(z_i)}{\sum_{j=1}^n \exp(z_j)},$$

for any  $z = (z_1, \dots, z_n) \in \mathbb{R}^n$  and  $i \in \{1, \dots, n\}$ . In other words,  $\text{argmin}^*(z) \approx \text{softmax}^*(-z)$  for each  $z = (z_1, \dots, z_n) \in \mathbb{R}^n$ . Thus, a differentiable approximation  $\tilde{E}: \Phi_n \rightarrow \mathbb{R}$  of the objective function  $E$  to be maximized is given by

$$\tilde{E}(\phi) = \frac{1}{|W|} \sum_{x \in W} \sum_{i=1}^n \lambda\left(\mathbb{1}_{C_i^{\text{GT}}}(x), \text{softmax}_i^*(-D(x, \phi))\right). \quad (9)$$

In particular, in [43], the similarity measure  $\lambda: \{0, 1\} \times [0, 1] \rightarrow (-\infty, 0]$  given by the negative binary cross-entropy loss  $\lambda(y, y') = y \log y' + (1 - y) \log(1 - y')$  is employed, where  $y \in \{0, 1\}$  and  $y' \in [0, 1]$ . Finally, to obtain the fitted GBPD model, the negative objective function  $-\tilde{E}$  is minimized using a (GPU-accelerated) stochastic gradient descent algorithm and running it for up to 25 iterations.

### 3.5 Gradient descent-based fitting II [Neper]

In [39], fitting Laguerre tessellations to data is formulated as a non-linear optimization problem, where the optimization variables are the coordinates and weights of the generators. For  $n$  generators, this leads to a total of  $4n$  variables. The approach, henceforth called Neper with reference to its implementation in the Neper package [55], was developed to account for statistical reconstruction of cell sizes and shapes. However, it can also be used for a grain-by-cell reconstruction based on microscopy measurements or 3D image data. Here, we use the latter.

The aim is to minimize the discrepancy between the measured grains and the cells of a Laguerre tessellation. To this end, for each  $i \in \{1, \dots, n\}$ , let

$$\partial C_i^{\text{GT}} = \{x \in C_i^{\text{GT}} : \min_{y \in \mathcal{N}_6(x)} \mathbb{1}_{C_i^{\text{GT}}}(y) = 0\}$$

denote the boundary voxels of cell  $C_i^{\text{GT}}$  with  $\mathcal{N}_6(x)$  denoting the set of voxels sharing a face with  $x$ . Again, it is useful to assume that  $V \subset \mathbb{R}^3$  is connected. The discrepancy of a grain  $C_i^{\text{GT}}$  and its corresponding Laguerre cell  $C_i$  can be defined via

$$\delta_i(\phi) = \sqrt{\sum_{x \in \partial C_i^{\text{GT}}} \inf\{\|x - y\|^2 : y \in C_i\}},$$

yielding the objective function  $\mathcal{O}: \Phi_n \rightarrow [0, \infty)$ , where

$$\mathcal{O}(\phi) = \frac{2}{\bar{d} \sum_{i=1}^n |\partial C_i^{\text{GT}}|} \sqrt{\sum_{i=1}^n \delta_i(\phi)^2},$$

with  $\bar{d}$  denoting the mean grain diameter in the grain map GT.

Minimizing  $\mathcal{O}(\phi)$  with respect to the variables  $x_1, \dots, x_n, w_1, \dots, w_n$  defines an unconstrained non-linear optimization problem. The implementation in Neper employs the C++ NLOpt library [56] to solve the problem using derivative-free methods: Subplex [57], a variant inspired by the Nelder–Mead simplex algorithm, and Praxis [58], which performs line minimization along principal axes. The initial parameter values are selected according to the heuristic Hq (see Section 3.1).

The optimization can terminate based on several criteria; following [39], we adopt an absolute error criterion, stopping when the improvement in the objective function over  $40n$  iterations falls below  $10^{-3}$ .

### 3.6 Other algorithms from the literature

#### 3.6.1 Gibbs-Laguerre tessellations

In [59], the reconstruction problem is addressed by generating a realization of an appropriate Gibbs point process. The point process distribution is governed by an energy function designed to minimize discrepancies between the Laguerre cells and the target distribution of grain characteristics. Various methods to incorporate correlations among these characteristics have also been developed [60]. While this approach has primarily been applied to stochastic reconstruction, it can be adapted to minimize discrepancies on a grain-by-cell basis. However, as the method is designed to match the geometric features of polyhedra, it does not readily apply to the reconstruction of voxel-based data.

#### 3.6.2 Gradient descent-based polyhedra matching

A further gradient descent-based method is described in [38]. Similarly to the method mentioned in Section 3.6.1, it relies on the polyhedral Laguerre cell representation. The objective is to minimize the total mismatch volume between the cells of the approximating tessellation and the observed grains. The total mismatch volume can be expressed in terms of a continuously differentiable function which needs to be minimized. The variables correspond to the set of generators.

#### 3.6.3 Optimal transport-based approaches

An optimal transport-based approach for generating Laguerre diagrams with prescribed cell volumes has been introduced in [48]. This approach is based on the result that, for any given set of cell volumes, a corresponding Laguerre tessellation exists, and finding such a tessellation reduces to solving a convex optimization problem. Although the primary focus is not on fitting, the authors demonstrate that the method can be adapted for this purpose by initializing the seed points at the centroids of the target grains. The subsequent work [61] proposes a method for generating a Laguerre diagram or GBPD with prescribed volumes whose centroids are close—in the least-squares sense—to a given set of target centroids. The paper [62] presents a highly efficient, GPU-accelerated implementation of a semidiscrete optimal transport method, accompanied by a Python library, for generating GBPDs with prescribed statistical properties.

#### 3.6.4 Simulated annealing approaches

The algorithm described in [40] and [44] is based on the simulated annealing optimization method, which draws inspiration from the physical annealing process. Starting from an initial parameter configuration, it iteratively perturbs a single parameter associated with a randomly selected generator, thereby producing an updated discrepancy value. The lower the new discrepancy, the higher the probability of the new parameter configuration being accepted. The speed of convergence can be controlled via a cooling schedule that is included in the acceptance probabilities.

### 3.7 Some general considerations

All methods discussed above fit a given grain structure using a tessellation from a specified model class. The quality of the fit is assessed—either directly or indirectly, as in the LP approach—using an

appropriate discrepancy metric, which is subsequently minimized with respect to the set of generators. For solving the optimization problem, iterative approaches such as the cross entropy method or gradient descent as well as a direct linear program can be used. In the literature, both volume-based and interface-based measures are considered, see the discussion in [41]. Volume-based measures aim at maximizing the volume overlap between the observed grains and their counterparts in the tessellation approximation. In contrast, interface-based measures only consider fitting the grain boundaries. Interface-based measures are more efficient from a computational point of view since only boundary voxels need to be checked. For Laguerre tessellations, the measures can additionally be evaluated analytically without discretizing the tessellation. For GBPDs this is currently not possible in 3D as no explicit representation of the cell boundaries is known, see [63] for the 2D case. To reduce the runtime further, the computation of the discrepancy measure can be reduced to a subset of voxels. This approach is applied by the CE method for the interface-based method and by LP when using the so-called *coresets* [45] in a volume-based approach.

In general, designing a fitting method can be viewed as a modular task that involves selecting (a) a class of tessellation models, (b) a data representation format, (c) a discrepancy measure, and (d) an optimization scheme—typically with associated hyperparameters. The performance of the optimization step can be further enhanced by specifying an appropriate initial configuration and, in many cases, a stopping criterion.

## 4 Image data

We evaluate several 3D polycrystal and foam image data sets to assess the performance of the algorithms stated in Section 3.

### 4.1 Polycrystals

#### 4.1.1 Time-resolved microstructure of AlCu polycrystals

We consider time-resolved 3D image data representing the polycrystalline microstructure of an aluminum (Al) copper (Cu) alloy. 3D imaging of a 1.4 mm-diameter cylinder of Al-5 wt%Cu has been performed by means of 3DXRD measurements as described in Section 3.2 of [64]. Image data has been acquired for seven different time steps during grain coarsening by Ostwald ripening. Each 3D image has a size of  $531 \times 321 \times 321$  voxels, where the cubic voxels have an edge length of  $5 \mu\text{m}$ . In the present paper, we focus on the data corresponding to the initial time step  $t = 0$ , as well as on data for  $t = 20$ , and  $t = 60$ . At the initial time, the image comprises 938 grains. Off-grid representations of the grain system by parametric tessellations such as Laguerre tessellations and GBPDs are discussed in [43], where the method described in Section 3.4 has been used to fit tessellation models to image data. Slices and a 3D rendering of the AlCu polycrystal data are shown in Figure 2. We will refer to these data sets as **AlCuStep0**, **AlCuStep20**, and **AlCuStep60**.

#### 4.1.2 Time-resolved microstructure of 99.9% pure iron polycrystals

We also consider time-resolved 3D image data representing the polycrystalline microstructure of a 99.9% pure iron sample. The data set is discussed and analyzed in detail in [8, 65], where the complete data processing workflow—from the initial experiment to the acquisition of grain scans—is thoroughly described, particularly within the supplementary materials. The data set, obtained by a diffraction contrast tomography (DCT) [66, 67] experiment at beamline ID11 at the European Synchrotron Radiation Facility (ESRF), comprises 15 3D images, which were taken at different time steps of an annealing process. The material was first cold-rolled and annealed for 30 minutes at  $700^\circ\text{C}$  to fully recrystallize before it was first scanned. In the present paper, we focus on the data for the initial time step  $t = 0$ . At this time step, the  $280 \times 320 \times 256$  voxel image, composed of cubic voxels each with an edge length of  $1.54 \mu\text{m}$ , contains a total of 1,327 grains. A 2D slice through this data is shown in Figure 3. We will refer to the data set as **PureFeStep0**.

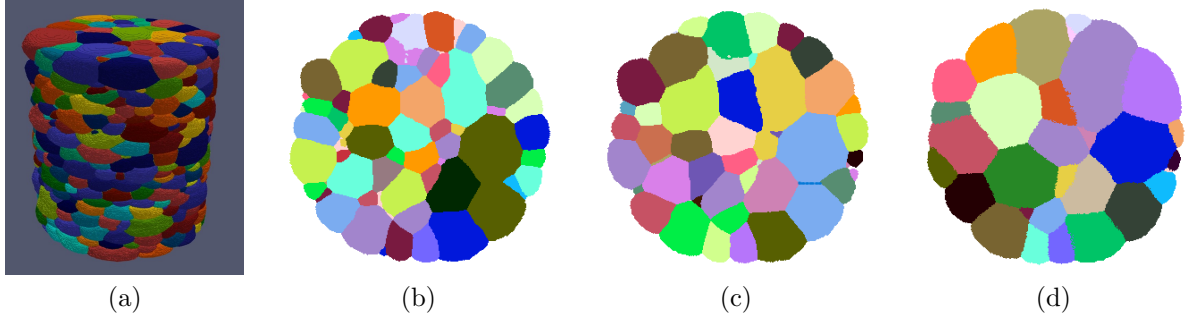


Figure 2: Image data representing grain growth in AlCu polycrystals, provided by C. E. Krill. A 3D rendering at the initial time step (a), as well as 2D cross-sections after time steps 0, 20, and 60 (b,c,d) are shown. The image size is  $531 \times 321 \times 321$  with a voxel edge length of  $5 \mu\text{m}$ .



Figure 3: 2D slice through the 3D dataset of 99.9% pure iron [22], provided by H. F. Poulsen. The image size is  $280 \times 320 \times 256$  with a voxel edge length of  $1.54 \mu\text{m}$ .

## 4.2 Foams

### 4.2.1 Ceramic foam

The first foam sample is a ceramic foam with a size of  $2.1 \text{ cm} \times 5 \text{ cm} \times 5 \text{ cm}$ . The pore size is 20 ppi (pores per inch). The sample was scanned by  $\mu\text{CT}$  at the Fraunhofer ITWM in Kaiserslautern, Germany, with a voxel edge length of  $33.91 \mu\text{m}$  resulting in an image size of approximately  $700 \times 1550 \times 1500$  voxels.

The wall system of this partially closed foam was segmented and analyzed in [68]. Stochastic models for the microstructure were presented in [69, 70]. A 2D slice of the ceramic foam image along with its segmentation is shown in Figure 4. Here, we consider a cropped section of the image of size  $400 \times 800 \times 800$  voxels that contains 1,003 pores. We will refer to the data set as **Ceramic**.

### 4.2.2 Closed polymer foam

The second example is a Rohacell<sup>®</sup> polymethacrylimide (PMI) closed-cell foam (WIND-F RC100) that was imaged by micro computed tomography with a voxel edge length of  $2.72 \mu\text{m}$ . The image size is  $1300 \times 1100 \times 1000$  voxels. Analysis of the image and Laguerre tessellation-based models for the 3D microstructure are presented in [47, 71]. A 2D slice of the polymer foam image and its segmentation are shown in Figure 5. Here, we consider a cropped section of the image of size  $600 \times 600 \times 600$  voxels that contains 380 pores. We will refer to the data set as **WIND**.



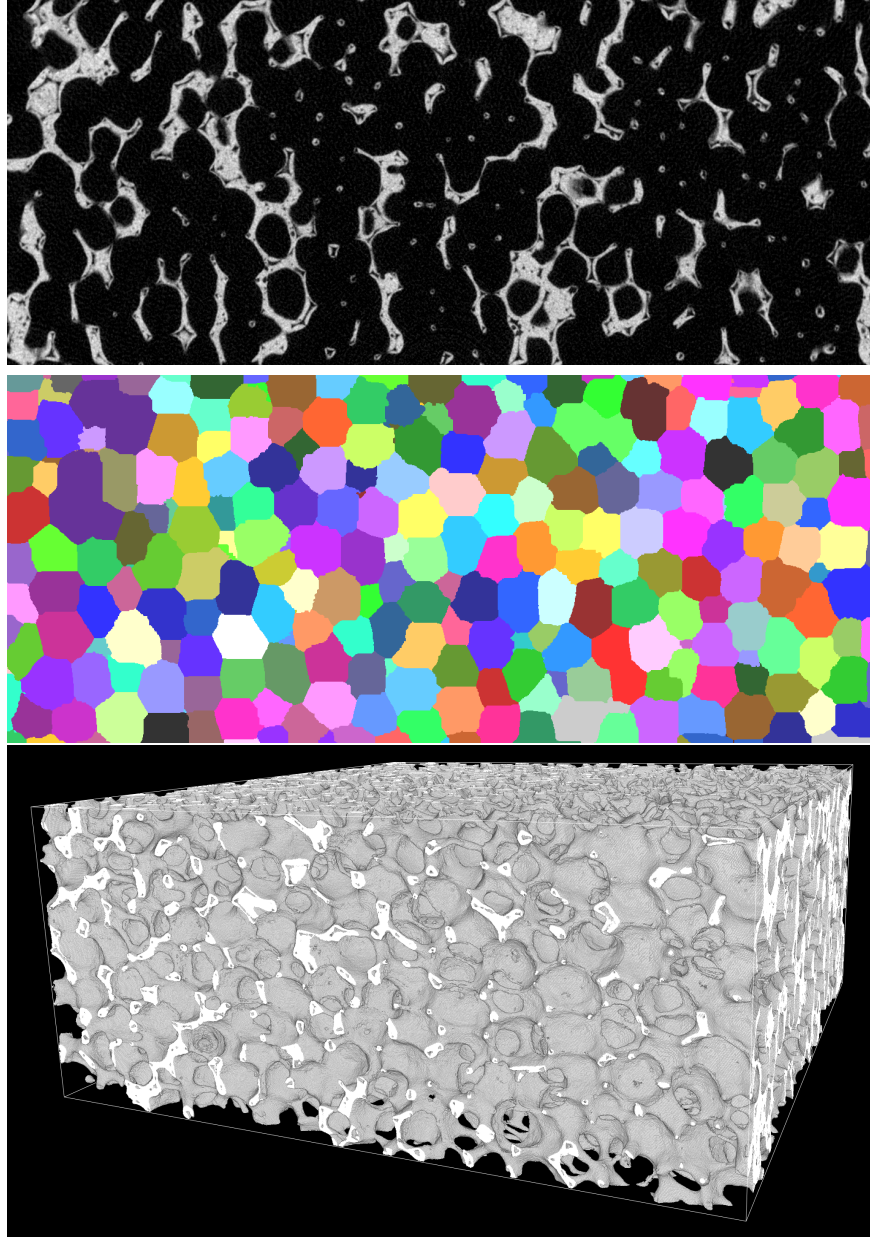


Figure 4: 2D slice of the reconstructed CT image of a partially closed ceramic foam (top), cell reconstruction by watershed (middle), and a volume rendering (bottom). The image size is  $700 \times 1550 \times 1500$  voxels with a voxel edge length of  $33.91 \mu\text{m}$ .

#### 4.2.3 Closed zinc foam

The closed zinc foam sample and its image are sourced from the project *Genormte Charakterisierung zellularer Werkstoffe mittels Computertomografie* (NORMZELL, BMWi funding reference 01FS11003). The image size is  $975 \times 1100 \times 1350$  voxels with a voxel edge length of  $18.95 \mu\text{m}$ . A slice of the zinc foam image along with its segmentation are shown in Figure 6. Here, we consider two cropped sections of the image, each of size  $400 \times 400 \times 400$  voxels, which contain 879 and 1,903 pores, respectively. The cropped cutouts are shown in Figure 7. We will refer to the data set as **Zinc1** and **Zinc2**.

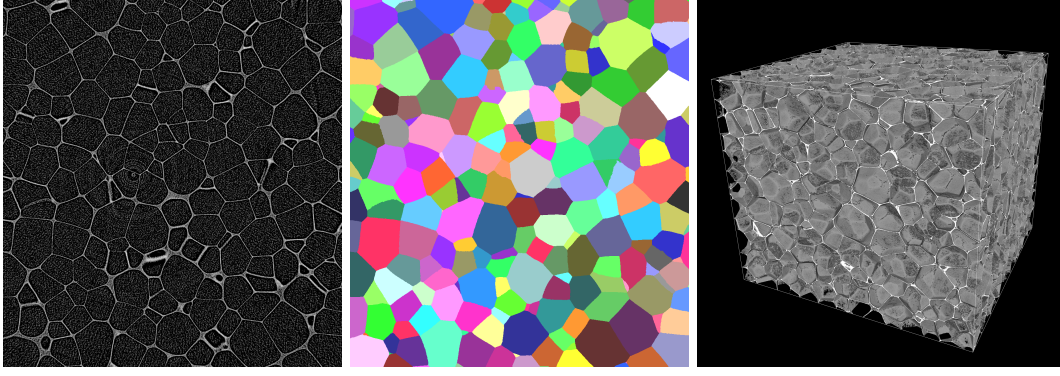


Figure 5: 2D slice of the reconstructed CT image of a closed polymer foam (left), cell reconstruction by watershed (middle), and a volume rendering (right). The image size is  $1300 \times 1100 \times 1000$  voxels with a voxel edge length of  $2.72 \mu\text{m}$ .

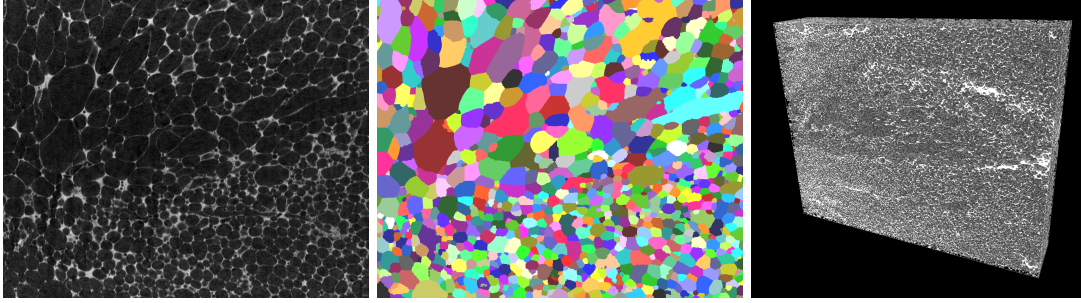


Figure 6: 2D slice of the reconstructed CT image of a closed zinc foam (left), cell reconstruction by watershed (middle), and a volume rendering (right). The image size is  $975 \times 1100 \times 1350$  voxels with a voxel edge length of  $18.95 \mu\text{m}$ .

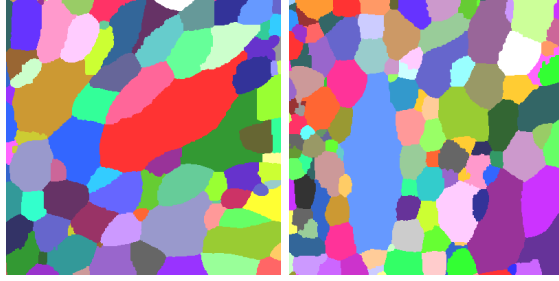


Figure 7: Cropped cutouts of the cell reconstruction shown in Figure 6 (middle), both of size  $400 \times 400 \times 400$  voxels. Left: Zinc1, right: Zinc2

## 5 Measures for performance evaluation

To assess the goodness of fit between the discretized tessellation cells  $C_1 = C_1(\phi) \cap W, \dots, C_n = C_n(\phi) \cap W$  and the ground truth  $\text{GT} : W \rightarrow \{0, \dots, n\}$ , representing  $n$  grains, we compute a range of performance measures. First, we consider the fraction  $F_c$  of correctly assigned voxels given by

$$F_c = \frac{1}{|\{x \in W : \text{GT}(x) > 0\}|} \sum_{i=1}^n |C_i^{\text{GT}} \cap C_i|.$$

Furthermore, we consider the relative frequency  $F_0 = n^{-1}|\{i \in \{1, \dots, n\}: C_i = \emptyset\}|$  of missing cells. The values for  $F_c$  and  $F_0$  for the fitting algorithms considered are listed in Tables 2 and 3 of the appendix, respectively.

In addition, we compute performance measures that quantify cell-wise discrepancies. From here on, we will restrict the comparison to non-missing cells. Therefore, we define the index set  $\mathcal{J} = \{i \in \{1, \dots, n\}: C_i \neq \emptyset\}$ . To characterize the shape and size of a cell  $C \subseteq W$ , we consider the volume-equivalent diameter  $\varphi_d(C)$  of  $C$ , which is given by

$$\varphi_d(C) = \sqrt[3]{\frac{6|C|}{\pi}},$$

as well as the surface area  $\varphi_A(C)$ , the elongation factor  $\varphi_{\text{elo}}(C)$  (ratio of second longest to longest half axes lengths of best fitting ellipsoid), and the flatness factor  $\varphi_{\text{flat}}(C)$  (ratio of shortest to second longest half axes lengths of best fitting ellipsoid) [72]. Then, for each descriptor  $\varphi \in \{\varphi_d, \varphi_A, \varphi_{\text{elo}}, \varphi_{\text{flat}}\}$  we quantify the mean normalized error of the fit by

$$F_\varphi = \frac{1}{|\mathcal{J}|\bar{\varphi}} \sum_{i \in \mathcal{J}} |\varphi(C_i^{\text{GT}}) - \varphi(C_i)|,$$

where  $\bar{\varphi} = \frac{1}{n} \sum_{i=1}^n \varphi(G_i^{\text{GT}})$ . The values of the performance measures  $F_{\varphi_d}$ ,  $F_{\varphi_A}$ ,  $F_{\varphi_{\text{elo}}}$ ,  $F_{\varphi_{\text{flat}}}$  for the considered fitting algorithms are given in Tables 4, 5, 6, and 7 of the appendix, respectively.

Furthermore, we define a performance measure to assess the accuracy with which the cells  $C_1, \dots, C_n$  of the fitted tessellation reflect the topology of GT. Therefore, for each  $i \in \mathcal{J}$ , let  $N^{\text{GT}}(i), N^T(i) \subseteq \{1, \dots, n\}$  denote the sets of indices of grains/cells adjacent to  $C_i^{\text{GT}}$  and  $C_i$  within the ground truth GT and the fitted tessellation, respectively, where the notion of adjacency is based on the  $\mathcal{N}_{26}$  neighborhood, as in Section 3.3. We then quantify the agreement between the neighborhood of  $C_i^{\text{GT}}$  and that of  $C_i$  using the intersection over union IoU( $i$ ) defined as

$$\text{IoU}(i) = \frac{|N^{\text{GT}}(i) \cap N^T(i)|}{|N^{\text{GT}}(i) \cup N^T(i)|}.$$

Finally, we quantify the goodness-of-fit with respect to the topology by the performance measure  $F_{\text{IoU}}$  which is given by

$$F_{\text{IoU}} = \frac{1}{|\mathcal{J}|} \sum_{i \in \mathcal{J}} \text{IoU}(i).$$

The values of  $F_{\text{IoU}}$  for the fitting algorithms considered are listed in Table 8 of the appendix.

## 6 Results

The values for the volume-based accuracy measure  $F_c$  listed in Table 2 indicate that many differences between the fitting algorithms considered in the present paper could be attributed to the choice of the tessellation model, rather than the fitting method. Overall, methods that fit GBPD-type tessellations generally achieve higher accuracies than those that fit Voronoi and Laguerre tessellations. This holds particularly for datasets that exhibit more complex cell morphologies (e.g., **Zinc1**, **PureFeStep0**). This is mostly to be expected because of the higher flexibility of GBPDs. However, for datasets that exhibit ‘simpler’ cell morphologies (e.g., convex cells), such as the **Ceramic** and **WIND** datasets, the algorithms that fit Laguerre tessellations already perform quite well. This could be attributed to the fact that Laguerre tessellations inherently enforce the constraint of planar cell facets. Among the algorithms that fit Laguerre tessellations, Neper yields the best accuracy values for the considered datasets. Notably, for the two datasets **Ceramic** and **WIND**, the fit achieved by the even simpler Voronoi tessellation yields results comparable to those of Laguerre tessellations fitted with Neper (see Table 2). As expected, for datasets that exhibit more complex grain architectures, the more general

Laguerre tessellation outperforms the Voronoi tessellation due to its greater flexibility in controlling cell sizes through an additional parameter per cell.

In total, GBPD tessellations fitted by the GD method, which fits all parameters, yield the best performance with respect to  $F_c$  for most of our datasets. In fact, across our datasets, the accuracy of the evaluated GBPD algorithms varies by no more than 5 percentage points. Interestingly, the Hq algorithm achieves the lowest mean normalized errors  $F_{\varphi_d}$  in volume-equivalent diameters across the evaluated data sets. This suggests that its underlying heuristic tends to generate tessellations whose cell volumes closely match those observed in the data. A similar trend was noted in [22], although that study also identified grain configurations for which Hq fails to produce satisfactory fits. In contrast, the LP method ensures that the generated GBPDs adhere to specified volume bounds, which were set to  $\pm 2$  voxels per grain in our experiments. When these bounds are reduced to zero, LP—unlike the other methods listed in Table 4—yields a volume-equivalent diameter error of  $F_{\varphi_d} = 0$  by construction.

The surface area errors  $F_{\varphi_A}$  in Table 5 show a similar trend as in Table 2. In particular, Laguerre tessellations have a limited capacity to reproduce the curved facets of the more complex data sets. Again, Laguerre tessellations fitted by Neper show a good (even the best) performance for the two foam data sets **Ceramic** and **WIND**.

The better ability of GBPDs to fit cell shapes is also evident from the errors  $F_{\varphi_{elo}}$  and  $F_{\varphi_{flat}}$  of the shape characteristics elongation and flatness, see Tables 6 and 7.

For almost all the considered datasets, Hq has the smallest frequency of missing cells, see Table 3. This can be explained by the fact that systems of non- or only mildly overlapping objects do not generate empty cells. Hence, the construction used in the heuristics—sites corresponding to the barycenters of the grains—is not prone to produce sets of generators with empty cells. The choice of update scheme in the iterative algorithms determines to which extent empty cells can arise in subsequent iterations.

With respect to topology, GBPDs outperform Laguerre tessellations again, see Table 8. The latter cannot reproduce neighborhood relations that require curved boundaries, see Figure 8.

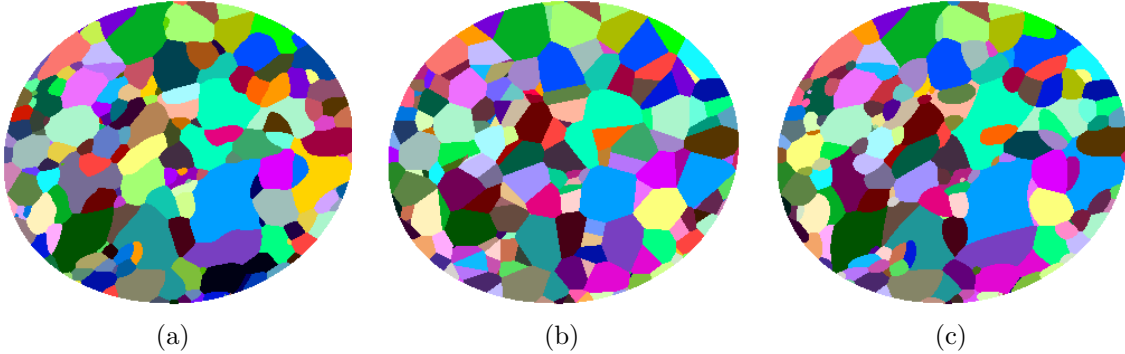


Figure 8: Fitting of the data set described in Section 4.1.2 using the method described in Section 3.4. Results are visualized by comparing image data (a), the fit with a Laguerre tessellation (b), and the fit of a GPBD (c) at the example of one 2D slice.

Cross sections of the data sets considered in this paper, together with a fitted Voronoi tessellation using GD, fitted Laguerre tessellations using Hq, Neper, CE and GD, a fitted diagonal GBPD using GD, and fitted GBPDs using GD, LP,  $H_0$  and Hq, are shown in Figures 9 to 16 of the appendix. A rough estimate of hardware-specific runtimes can be found, for example, in [43].

## 7 Summary

We reviewed various algorithms for fitting Voronoi tessellations, Laguerre tessellations and GBPDs to grain structures observed in polycrystalline materials and foams. The effectiveness of these algorithms varied depending on the specific data sets, the tessellation models employed, and the evaluation criteria

used. The heuristic Hq achieved good performance on our data sets while incurring small computational cost. However, this is not always the case—as illustrated in [62], where the relative error in the resulting areas reaches 380%, and in [22], which highlights substantial differences between Hq and  $H_0$ . Nevertheless, due to its very low computational cost, Hq seems a useful choice for generating initial configurations for further optimization. Each of the presented algorithms exhibits distinct characteristics, and in practical applications, one must determine which of these are most suitable for the specific use case. The modular structure of the proposed fitting approaches enables targeted improvements, such as enhancing the accuracy of surface area or volume representations. The established discrepancy metrics primarily account for mismatches in cell volumes and boundaries. Additionally, metrics related to cell shape and topology—used here for model validation—can also be incorporated directly into the fitting process. This flexibility allows for the development of application-specific fitting strategies tailored to the structural features of interest.

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## Appendix

	Voronoi	Laguerre				d-GBPD	GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H <sub>0</sub>	Hq
<b>AlCuStep0</b>	0.80	0.88	0.93	0.86	0.85	0.93	<b>0.95</b>	0.90	0.93	0.93
<b>AlCuStep20</b>	0.82	0.89	0.94	0.88	0.86	0.94	<b>0.95</b>	0.93	0.94	0.94
<b>AlCuStep60</b>	0.82	0.89	0.93	0.90	0.85	0.94	<b>0.96</b>	0.93	0.94	0.94
<b>PureFeStep0</b>	0.68	0.69	0.73	0.62	0.71	0.80	<b>0.90</b>	0.85	0.85	0.86
<b>Ceramic</b>	0.91	0.89	0.92	0.91	0.91	<b>0.93</b>	0.90	<b>0.93</b>	0.92	0.92
<b>WIND</b>	0.90	0.88	0.94	0.93	0.92	<b>0.96</b>	0.94	0.93	0.93	0.93
<b>Zinc1</b>	0.74	0.74	0.80	0.74	0.77	0.86	<b>0.92</b>	0.90	0.89	0.90
<b>Zinc2</b>	0.76	0.80	0.83	0.79	0.80	0.89	<b>0.91</b>	<b>0.91</b>	0.90	0.90

Table 2: Values of  $F_c$  achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre				d-GBPD	GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H <sub>0</sub>	Hq
AlCuStep0	0.01	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	0.02	0.09	<b>0.00</b>	0.12	<b>0.00</b>	<b>0.00</b>
AlCuStep20	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	0.01	0.10	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>
AlCuStep60	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	0.11	<b>0.00</b>	0.05	<b>0.00</b>	<b>0.00</b>
PureFeStep0	0.01	0.02	0.04	0.03	0.02	0.08	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>
Ceramic	0.01	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	0.01	<b>0.00</b>	0.01	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>
WIND	0.04	0.01	<b>0.00</b>	<b>0.00</b>	0.07	<b>0.00</b>	0.02	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>
Zinc1	0.01	0.01	0.02	0.02	0.02	0.19	<b>0.00</b>	0.07	<b>0.00</b>	<b>0.00</b>
Zinc2	0.01	<b>0.00</b>	0.01	<b>0.00</b>	0.01	0.12	<b>0.00</b>	0.05	<b>0.00</b>	<b>0.00</b>

Table 3: Values of  $F_0$  achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre				d-GBPD	GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H <sub>0</sub>	Hq
AlCuStep0	0.104	0.069	0.015	0.036	0.067	0.032	0.017	0.068	0.012	<b>0.011</b>
AlCuStep20	0.093	0.065	0.017	0.033	0.062	0.024	0.015	0.013	0.012	<b>0.011</b>
AlCuStep60	0.094	0.071	0.021	0.039	0.071	0.023	0.014	0.048	0.012	<b>0.011</b>
PureFeStep0	0.153	0.128	0.082	0.149	0.115	0.051	0.025	0.059	0.029	<b>0.022</b>
Ceramic	0.016	0.046	<b>0.008</b>	0.010	0.010	0.014	0.030	0.014	0.014	0.009
WIND	0.053	0.079	0.014	0.040	0.025	0.020	0.024	0.016	0.016	<b>0.012</b>
Zinc1	0.141	0.127	0.044	0.101	0.098	0.055	0.025	0.037	0.025	<b>0.019</b>
Zinc2	0.113	0.090	0.037	0.071	0.081	0.046	0.029	0.041	0.021	<b>0.016</b>

Table 4: Values of  $F_{\varphi_d}$  achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre				d-GBPD	GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H <sub>0</sub>	Hq
AlCuStep0	0.238	0.122	0.065	0.074	0.171	0.066	0.042	0.142	<b>0.034</b>	0.040
AlCuStep20	0.215	0.115	0.066	0.068	0.158	0.057	0.037	<b>0.035</b>	<b>0.035</b>	0.039
AlCuStep60	0.234	0.188	0.140	0.138	0.194	<b>0.103</b>	0.107	0.127	0.111	0.111
PureFeStep0	0.347	0.235	0.164	0.239	0.289	0.137	0.066	0.100	0.058	<b>0.053</b>
Ceramic	0.077	0.105	<b>0.073</b>	0.077	0.074	0.076	0.086	0.075	0.077	0.079
WIND	0.095	0.091	<b>0.028</b>	0.048	0.062	0.038	0.053	0.037	0.037	0.039
Zinc1	0.288	0.232	0.128	0.190	0.225	0.115	<b>0.072</b>	0.091	0.111	0.110
Zinc2	0.268	0.196	0.132	0.170	0.212	0.104	<b>0.084</b>	0.100	0.107	0.103

Table 5: Values of  $F_{\varphi_A}$  achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre			d-GBPD		GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H <sub>0</sub>	Hq
AlCuStep0	0.176	0.112	0.106	0.109	0.153	0.072	0.043	0.059	<b>0.029</b>	0.030
AlCuStep20	0.174	0.102	0.106	0.098	0.160	0.057	0.040	0.034	<b>0.030</b>	<b>0.030</b>
AlCuStep60	0.174	0.119	0.118	0.111	0.155	0.056	0.036	0.045	0.033	<b>0.032</b>
PureFeStep0	0.245	0.229	0.230	0.235	0.227	0.131	<b>0.059</b>	0.072	0.068	0.066
Ceramic	0.071	0.165	0.068	0.085	0.073	0.049	0.073	<b>0.037</b>	0.040	0.038
WIND	0.110	0.190	0.092	0.096	0.085	<b>0.056</b>	0.059	0.059	0.063	0.060
Zinc1	0.220	0.207	0.212	0.202	0.209	0.109	0.060	<b>0.054</b>	0.059	0.058
Zinc2	0.198	0.179	0.165	0.177	0.176	0.085	0.068	<b>0.054</b>	0.056	0.055

Table 6: Values of  $F_{\varphi_{\text{elo}}}$  achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre			d-GBPD		GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H <sub>0</sub>	Hq
AlCuStep0	0.159	0.113	0.087	0.097	0.143	0.071	0.044	0.056	<b>0.031</b>	0.032
AlCuStep20	0.147	0.116	0.094	0.103	0.140	0.060	0.043	0.032	<b>0.029</b>	0.030
AlCuStep60	0.156	0.122	0.099	0.101	0.139	0.058	0.044	0.042	<b>0.030</b>	<b>0.030</b>
PureFeStep0	0.257	0.264	0.227	0.254	0.247	0.159	<b>0.066</b>	0.071	0.068	<b>0.066</b>
Ceramic	0.098	0.137	0.088	0.103	0.098	0.060	0.087	<b>0.048</b>	<b>0.048</b>	0.049
WIND	0.106	0.148	0.096	0.090	0.089	0.068	0.080	<b>0.061</b>	0.062	0.062
Zinc1	0.251	0.249	0.239	0.251	0.247	0.141	0.078	0.059	<b>0.058</b>	<b>0.058</b>
Zinc2	0.189	0.161	0.161	0.177	0.171	0.089	0.076	0.053	<b>0.051</b>	<b>0.051</b>

Table 7: Values of  $F_{\varphi_{\text{flat}}}$  achieved by deploying the considered fitting methods to the different data sets.

	Voronoi	Laguerre			d-GBPD		GBPD			
	GD	Hq	Neper	CE	GD	GD	GD	LP	H <sub>0</sub>	Hq
AlCuStep0	0.750	0.862	0.903	0.879	0.824	0.854	<b>0.945</b>	0.820	<b>0.945</b>	0.938
AlCuStep20	0.798	0.875	0.911	0.890	0.843	0.874	<b>0.959</b>	0.946	0.948	0.946
AlCuStep60	0.806	0.874	0.913	0.886	0.855	0.871	<b>0.949</b>	0.866	0.939	0.938
PureFeStep0	0.660	0.689	0.714	0.519	0.718	0.754	0.880	0.838	0.879	<b>0.881</b>
Ceramic	0.935	0.882	0.944	0.919	0.936	0.954	0.928	0.950	<b>0.955</b>	0.949
WIND	0.874	0.843	0.910	0.880	0.920	<b>0.928</b>	0.903	0.912	0.916	0.902
Zinc1	0.698	0.733	0.789	0.689	0.761	0.738	0.900	0.865	<b>0.905</b>	0.901
Zinc2	0.722	0.787	0.833	0.757	0.787	0.810	0.903	0.885	<b>0.917</b>	0.912

Table 8: Values of  $F_{\text{IoU}}$  achieved by deploying the considered fitting methods to the different data sets.

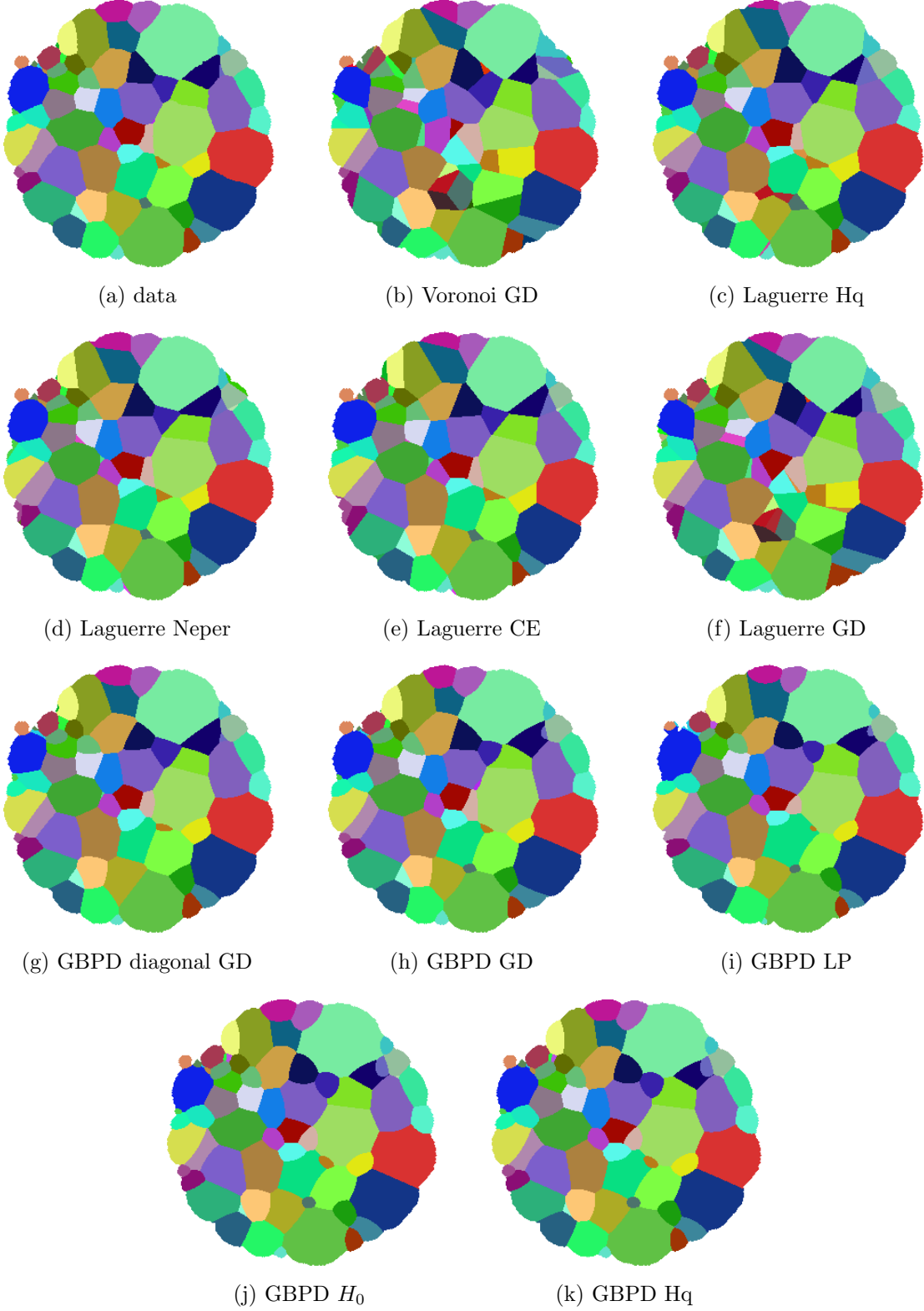


Figure 9: Cross sections of the **AlCuStep0** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using  $H_q$  (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i),  $H_0$  (j) and  $H_q$  (k).

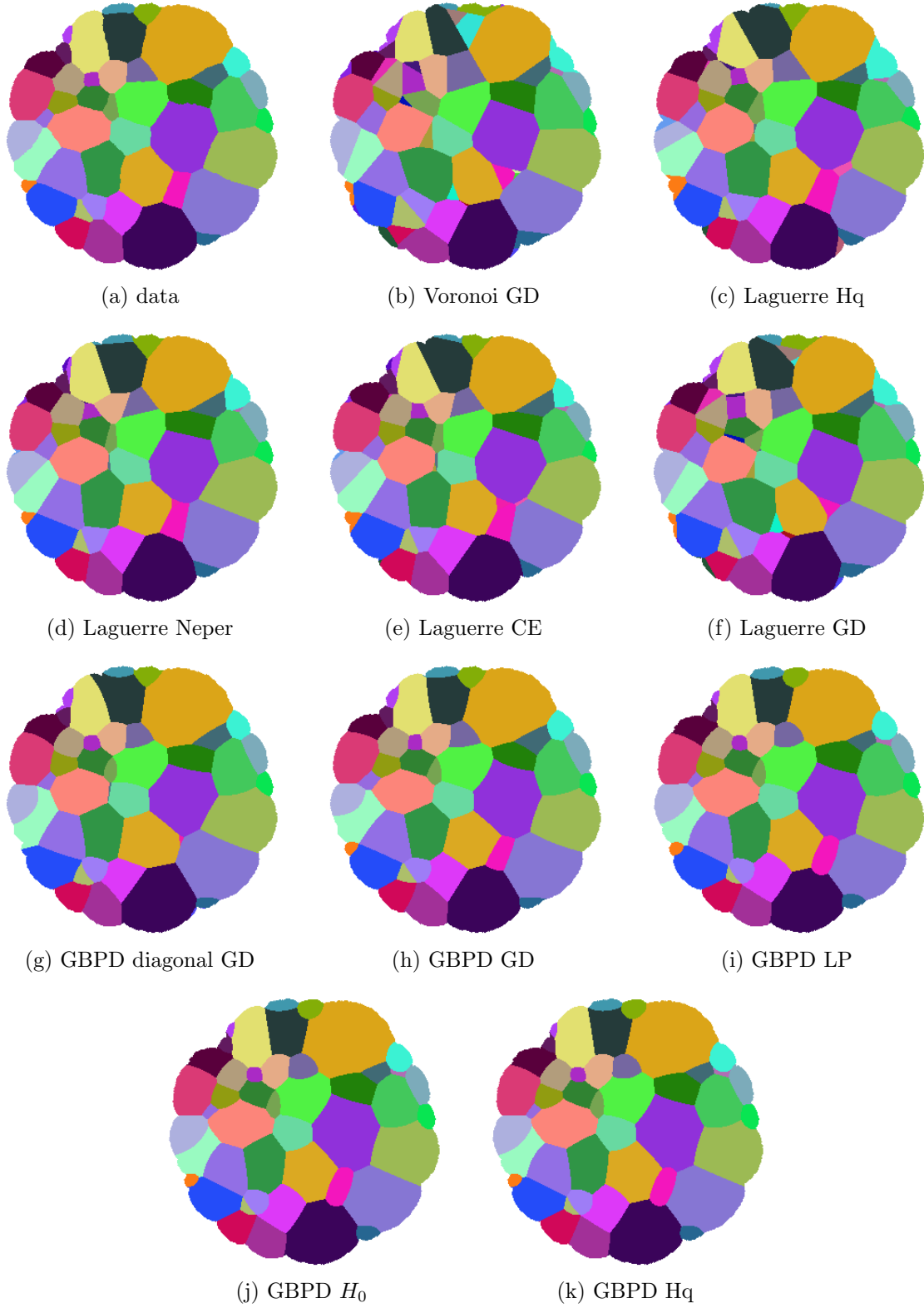


Figure 10: Cross sections of the **AlCuStep20** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using  $H_q$  (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i),  $H_0$  (j) and  $H_q$  (k).

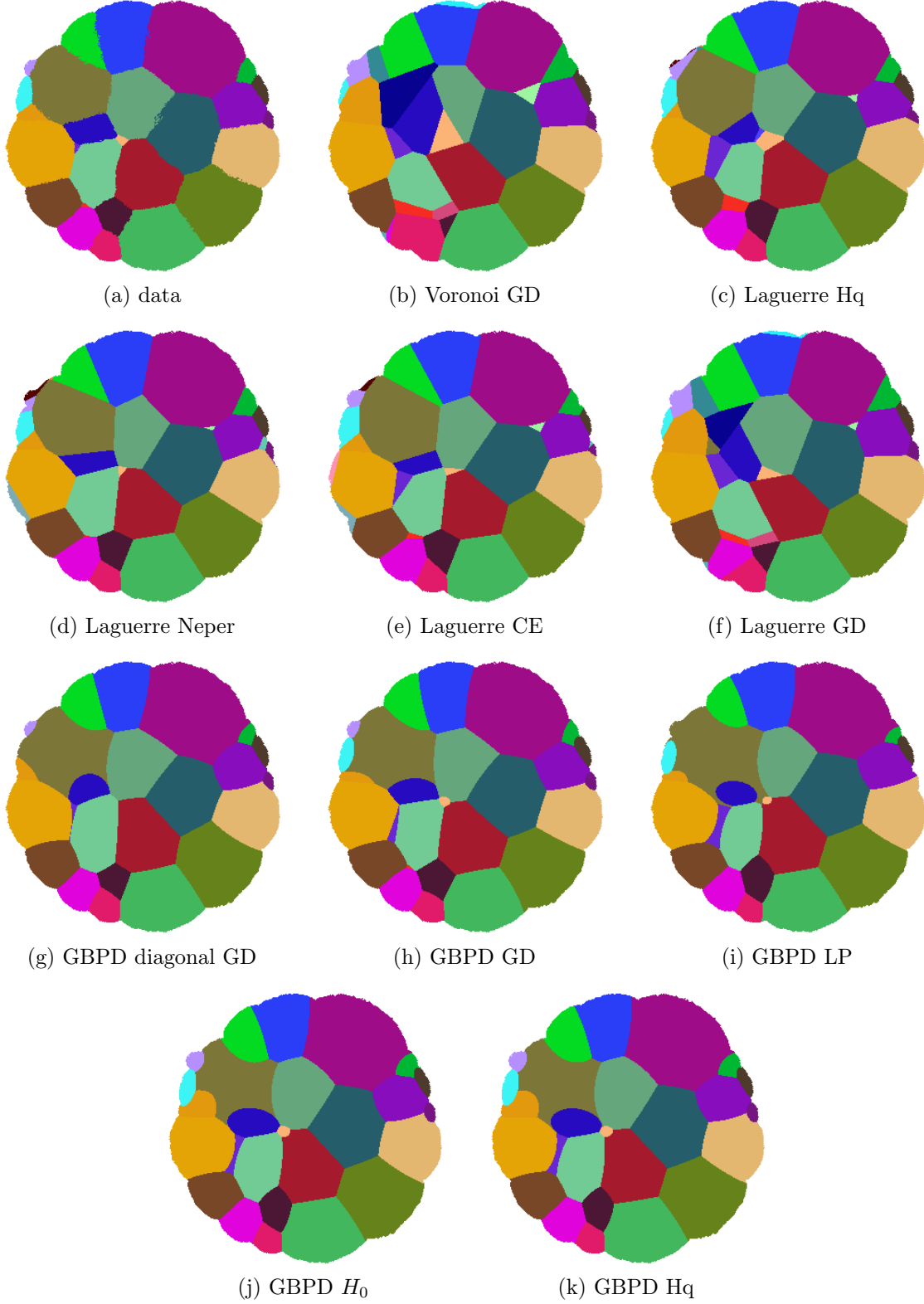


Figure 11: Cross sections of the **AlCuStep60** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i),  $H_0$  (j) and  $H_q$  (k).

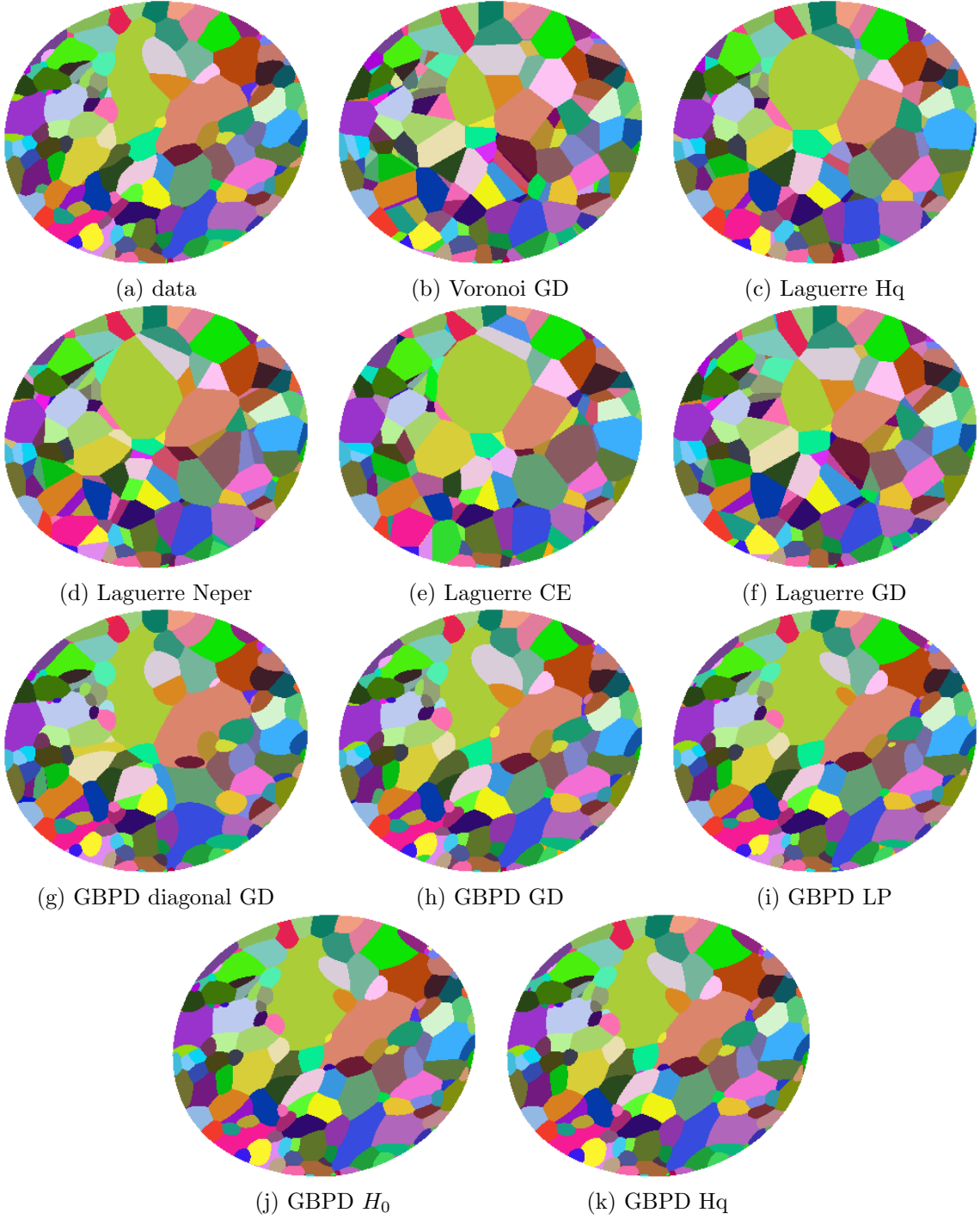


Figure 12: Cross sections of the **PureFeStep0** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i),  $H_0$  (j) and Hq (k).

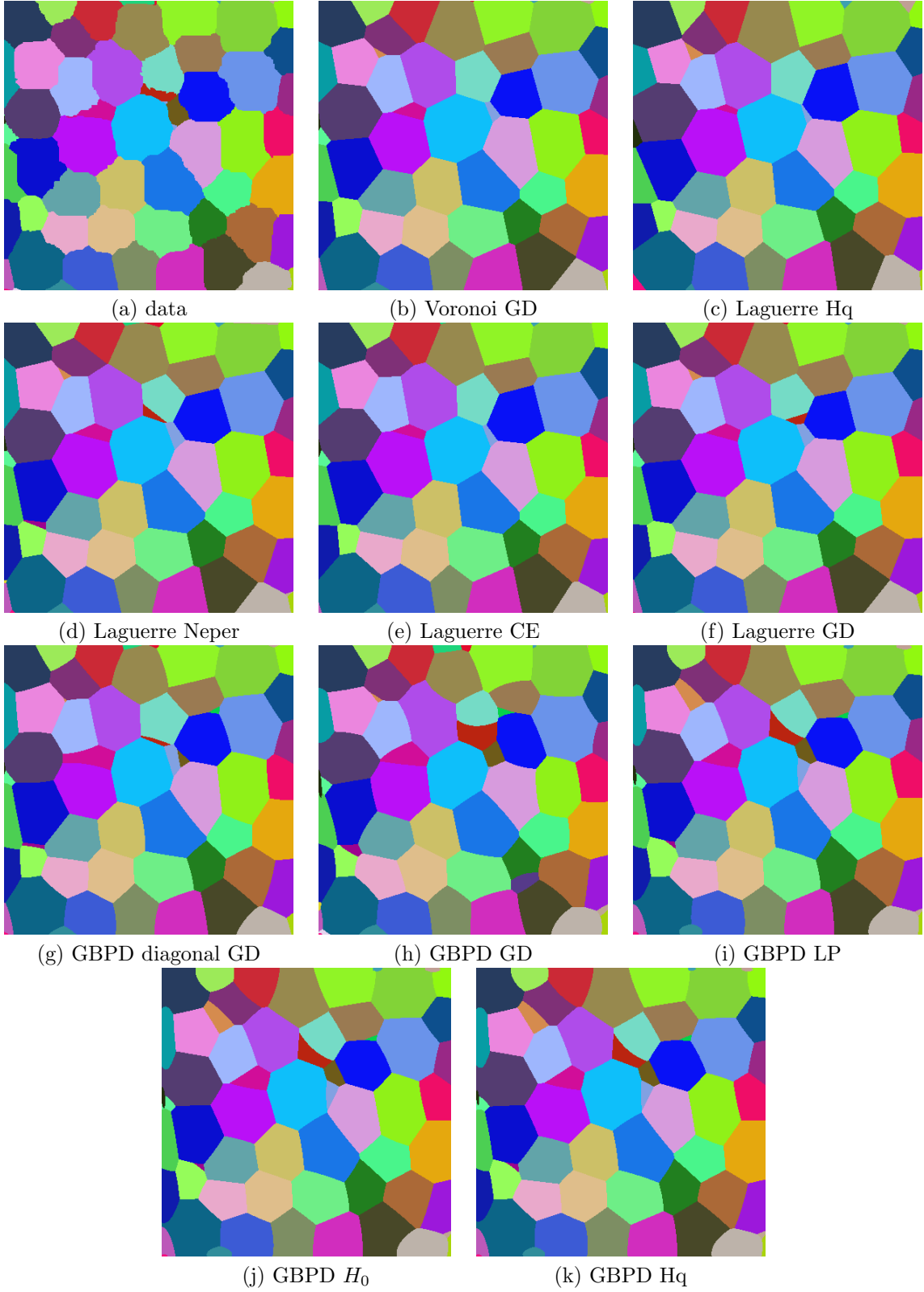


Figure 13: Cross sections of the **Vesuvius** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i),  $H_0$  (j) and  $H_q$  (k).



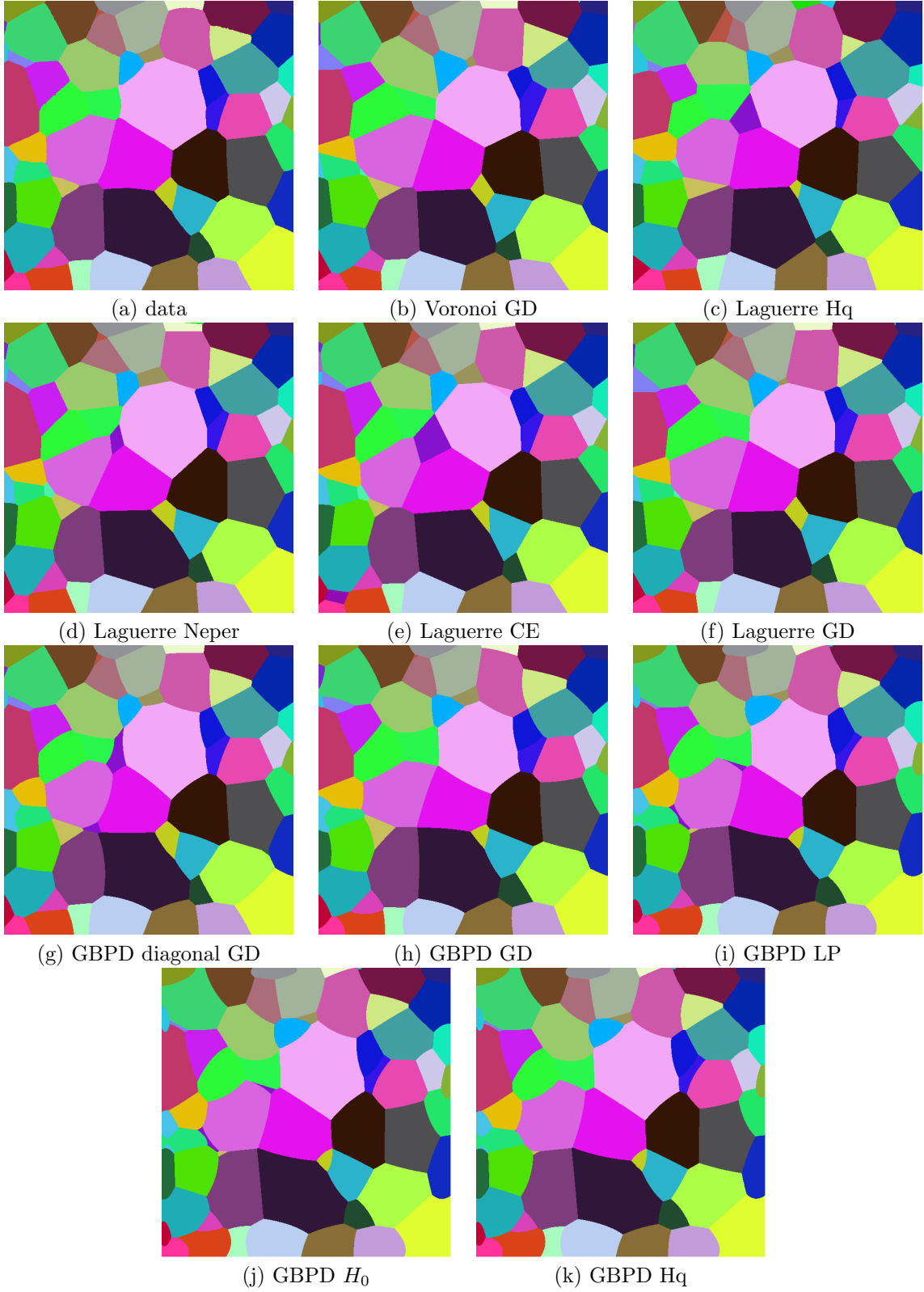


Figure 14: Cross sections of the **WIND** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i),  $H_0$  (j) and  $H_q$  (k).

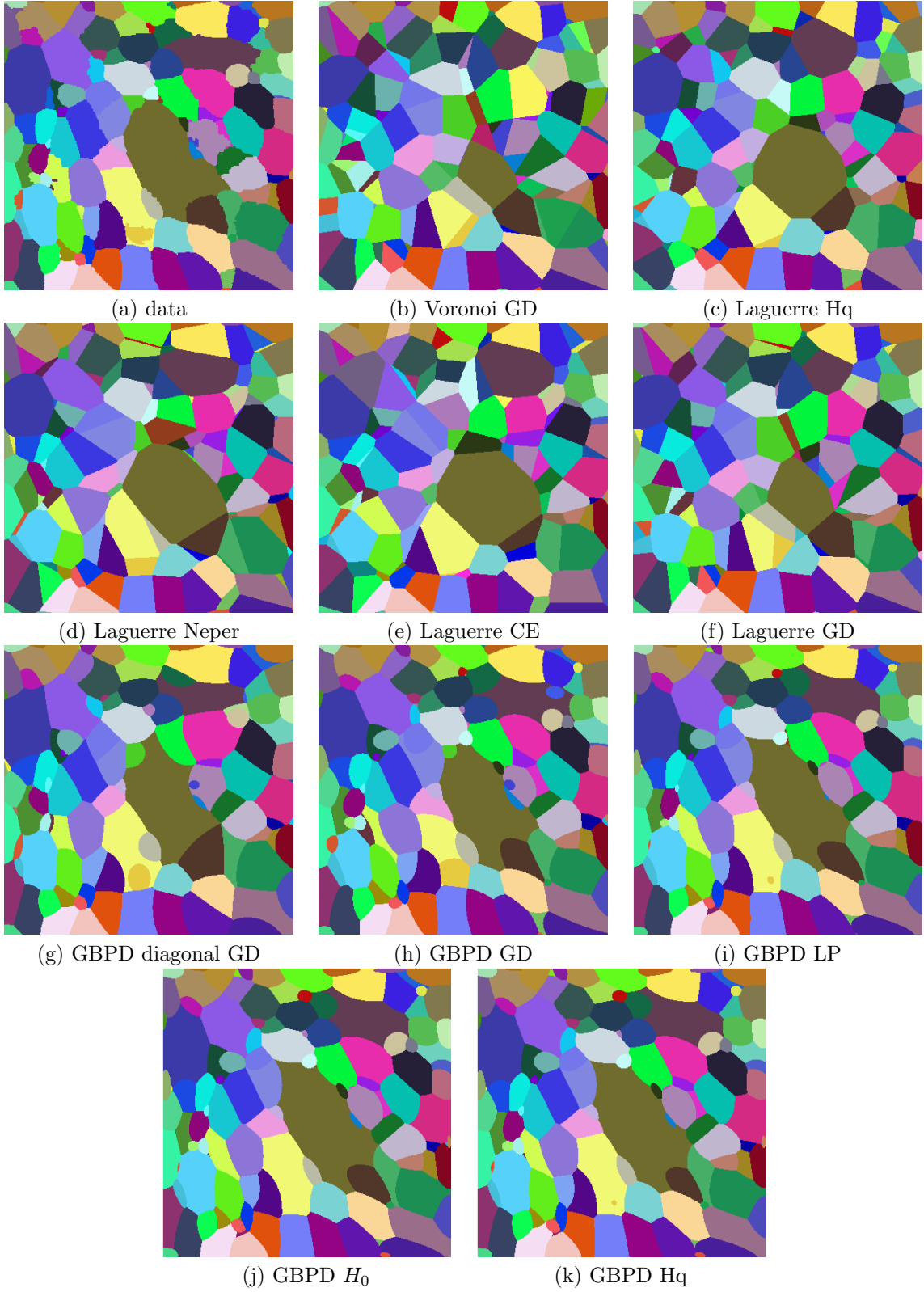


Figure 15: Cross sections of the **grillo063-879** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i),  $H_0$  (j) and  $H_q$  (k).

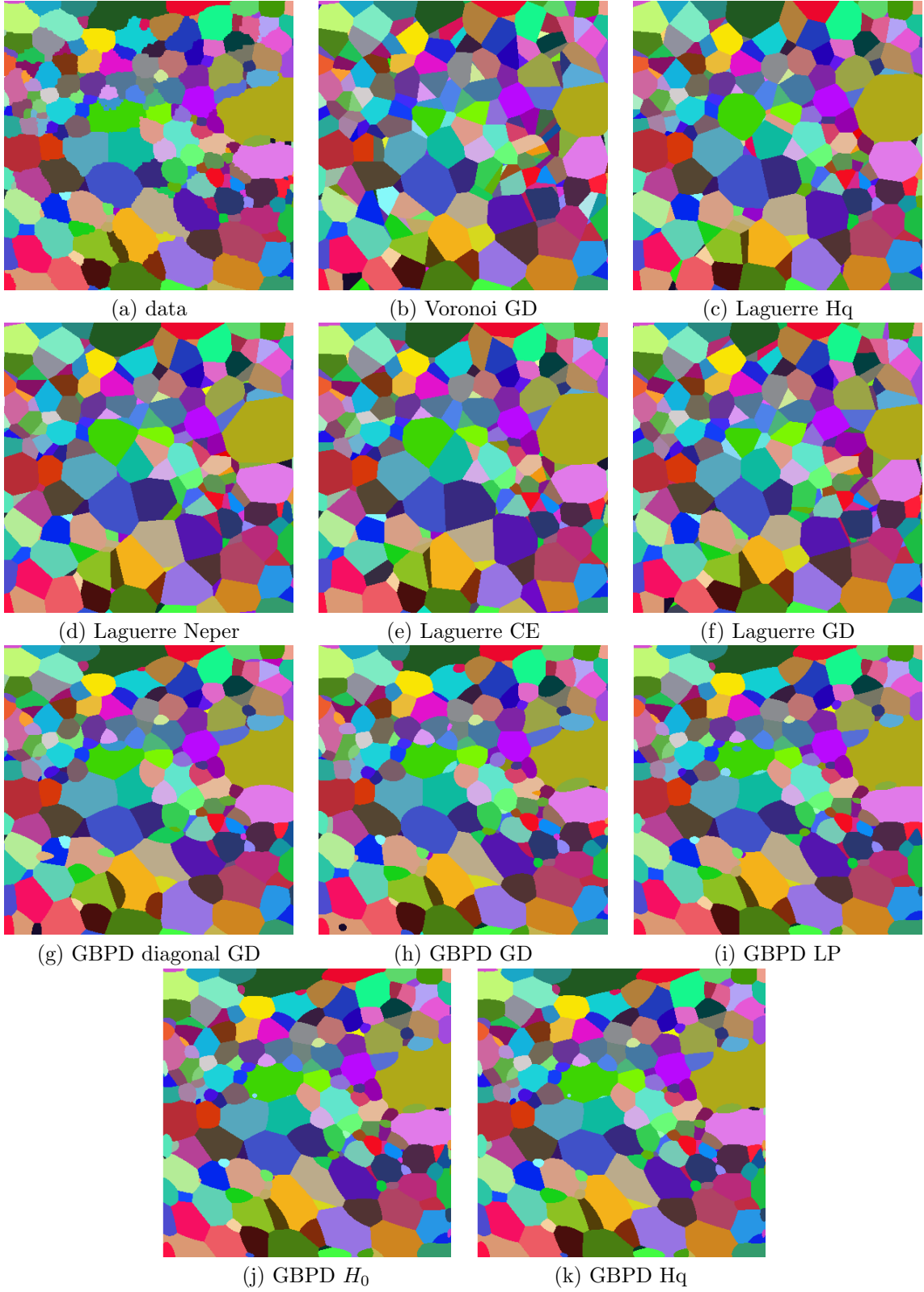


Figure 16: Cross sections of the **grillo063-1903** data set (a), a fitted Voronoi tessellation using GD (b), fitted Laguerre tessellations using Hq (c), Neper (d), CE (e) and GD (f), a fitted diagonal GBPD using GD (g), and fitted GBPDs using GD (h), LP (i),  $H_0$  (j) and  $H_q$  (k).