Abstract

Given a system of closed convex domains (inclusions) in $n$ dimensional Euclidean space, new computational meshes are introduced which partition the convex hull of the inclusion set into simple geometric objects. These partitions generalize the concept of Delaunay triangulations by interpreting the inclusions as generalized vertices while the remaining elements of the partition serve as connections between generalized vertices and therefore assume the classical role of edges, faces, etc. The proposed partitions are derived in two different ways: by exploiting duality with respect to certain generalized Voronoi partitions and by generalizing the well known Delaunay (empty circumcircle) criterion.

Generalized Delaunay partitions are of practical importance for the modeling of particle- and fiber-reinforced composite materials since they enable an efficient conforming resolution of the highly complicated component geometries. The number of elements in the partitions is proportional to the number of inclusions which is minimal.

Keywords: Delaunay triangulation, Euclidean (weighted) Voronoi diagram, conforming partition, composite material.

1. Introduction

The Voronoi tessellation [24] and the Delaunay triangulation [8] are well known (dual) concepts to study the geometry and topology of a system (finite set) of points. Voronoi tessellations generalize to systems of sets in a natural way as it will be described later. Generalization of Delaunay triangulation, however, are not straightforward in this context. In this paper, we introduce generalized partitions which preserve duality with respect to corresponding Voronoi tessellations. Our studies are strongly motivated by the investigation of particle-reinforced composite materials.

Composite materials (or composites for short) are engineered materials made from two or more constituent materials with significantly different physical properties. In a typical configuration, (hard) filler particles (reinforcement, inclusions) are surrounded by a matrix of a second material which binds the filler particles together. Because the characteristics and relative volumes of both the matrix material and the various filler particles can be manipulated, these materials show an almost infinite range of physical properties. As a representative model problem we consider the computation of heat distributions in particle-reinforced composites and their effective conductivities. Consider, e.g., packagings of integrated circuits that need to combine stability and light weight built with high conductivity for cooling purposes; a typical configuration

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is a background material (matrix) based on an epoxy based polymer providing the mechanical properties with tiny ceramic inclusions (filler) providing sufficient heat conductivity.

A model for the latter setting reads as follows. Let $\mathcal{F} = \{I_1, I_2, \ldots, I_N\}$ be a system of closed convex subsets of some bounded domain $\Omega \subseteq \mathbb{R}^n$, $n \in \mathbb{N} = \{1, 2, \ldots\}$. In the present context, the so-called inclusions $I \in \mathcal{F}$ have a larger characteristic conductivity than the surrounding material. Mathematically, we consider the boundary value problem

$$
- \text{div}(c \nabla u) = f \quad \text{in} \quad \Omega, \quad u = u_0 \quad \text{on} \quad \text{bnd}(\Omega), \quad (1)
$$

where $u_0$ is a given heat distribution on the boundary of the medium, and $f$ is some heat density. The major difficulty is hidden in the coefficient function $c$ representing the different conductivities of the constituent materials:

$$
c(x) = \begin{cases} 
1, & x \in \Omega \setminus \bigcup \mathcal{F}, \\
c_{\text{cont}} > 1, & x \in \bigcup \mathcal{F};
\end{cases} \quad (2)
$$

c_{\text{cont}} \gg 1$ being a constant that represents the conductivity contrast in the medium. The critical (large) parameters in this context are the number of inclusions $N$ and the conductivity contrast $c_{\text{cont}}$. A geometry of the coefficient $c$ of a particle-reinforced composite with circular inclusions of varying diameters in the unit square is depicted in Figure 1. Apart from convexity and closeness there are no restrictions on the inclusions in $\mathcal{F}$. The inclusions are not assumed to be pairwise disjoint, they even might even overlap on lower dimensional manifolds allowing to model inclusions that touch. Furthermore, certain non-convex inclusions (see (6)) can be modeled as finite unions of convex ones, without discussing this situation in detail within this article.

The numerical solution of problem (1) with coefficient (2) using a state-of-the-art method, e.g. a finite element method, requires a special treatment of the jumps of the coefficient which might cause discontinuities in the solution gradient. Our strategy is to encode the coefficient discontinuities explicitly in the computational partitions. Partitions which exactly resolve the interfaces between different material components by its elements, i.e. edges, faces, etc., are called conforming. Their great advantage is that important geometric parameters such as the volume fraction, i.e. the quotient of filler and matrix volumes, are exactly preserved. Moreover, the discretization error, typically, does not depend on the conductivity contrast. However, the computation of standard polygonal meshes that fulfill such a conformity constraint (at least approximately) is a major difficulty; see e.g. Section 2 in [10] on constraint triangulations and references therein. In addition, a conforming polygonal mesh can be poor (with regard to the shape regularity of its elements) or hardly available on standard computers in cases where the number of such coefficient jumps becomes critically large as it is the case in (1).

In this article we describe an efficient way of partitioning $\Omega$ coformingly into elements that are explicitly parametrizable and that can be represented by only few ($O(1)$) data which enables their easy use in further finite element computations. Inspired by the triangle-neck partition that has been used for modeling composites with equally sized circular inclusions [5] and spherical inclusions [4], we introduce the generalized Delaunay partition. As in the example of circular inclusions in the plane depicted in Figure 1, the inclusions will assume the classical role of vertices; two neighboring inclusions will be connected by channel-like objects and any three neighboring inclusions will induce a triangle in the 2-dimensional setting. By definition, the resulting partition is conforming. The number of elements is proportional to the number of inclusions which is minimal. We present a general theory of the aforementioned generalized Delaunay partitions including

1. the treatment of general, possibly overlapping, convex inclusions,
2. a multi-dimensional setting, and
3. the investigation of combinatorial structures in alignment with a concept of duality with respect to its corresponding Voronoi partitions.

Outline. Section 2 is devoted to the investigation of Voronoi partitions with respect to systems of sets which generalize ordinary planar Voronoi tessellations. These Voronoi partitions, i.e. subdivisions of $\mathbb{R}^n$ into regions reflecting proximity with respect to the inclusions, are the basis for the first definition of generalized Delaunay partitions stated in Section 3. A second characterization of generalized Delaunay partitions will follow up. Thereby the well-known Delaunay criterion is generalized. Equivalence of both definitions is shown. The analysis is illustrated by several figures. A short conclusion with references to future research will close this article.

Notation. In this paper we will use capital letters ($A, B, C, \ldots$) to indicate sets, bold letters ($\mathbf{x}, \mathbf{y}, \mathbf{z}, \ldots$) will indicate points in $n$-dimensional Euclidean space. Systems of sets will be denoted by calligraphic capital letters ($\mathscr{I}, \mathscr{P}, \ldots$) with the only exception of the power set of a set (denoted by $\mathcal{P}$). For systems of sets $\mathscr{I}$ we will denote the union of its elements by $\bigcup \mathscr{I} := \bigcup_{I \in \mathscr{I}} I$. We further make use of basic topological notations: For any subset $X$ of a metric space we denote its closure by $\text{cl}(X)$, its interior by $\text{int}(X)$, its relative interior by $\text{relint}(X)$, and its boundary by $\text{bnd}(X)$. Given a mapping $f$ from a set $A$ onto a set $B$ we will denote by $f^{-1}$ the mapping from $f(A) \subseteq B$ into $\mathcal{P}(A)$ that assigns to every $b \in B$ its preimage.

2. Generalized Voronoi partitions

We will first fix our notion of a partition.
Definition 1. As a partition $\mathcal{P} = \mathcal{P}(X)$ of a set $X$ we consider any subdivision of $X$ into finitely many non-overlapping subsets that cover all of $X$. More precisely,

$$P \cap Q = \emptyset, \forall P \neq Q \in \mathcal{P} \quad \text{and} \quad \bigcup_{P \in \mathcal{P}} P = X. \quad (3)$$

We will refer to $P \in \mathcal{P}(X)$ as an element of the partition $\mathcal{P}(X)$.

Note that $\mathcal{P}(X)$ is contained in the power set $\mathcal{P}(X)$ of $X$. In what follows the set $X$, which will be partitioned, is supposed to be a subset of $\mathbb{R}^n$ for some $n \in \mathbb{N}$. With regard to practical applications we consider the standard Euclidean setting rather than embedding the discussion in general metric spaces, i.e. we consider $\mathbb{R}^n$ equipped with Euclidean norm $\| \cdot \|$ and its induced metric $\text{dist}(\cdot, \cdot)$ given by

$$\|x\| := \sqrt{\sum_{i=1}^{n} x_i^2}, \quad \text{dist}(x, y) := \|x - y\|, \quad x, y \in \mathbb{R}^n. \quad (4)$$

The classical Voronoi partition [24] is a well known and intuitive concept to tessellate the space. It has been studied intensively over the last century, both, theoretically and computationally. Surveys from different points of view are provided by the book of Okabe and co-authors [19], the articles of Aurenhammer [2], Aurenhammer and Klein [3] and to the books of Preparata and Shamos [22] and Edelsbrunner [10]. Furthermore, nearly any textbook on computational geometry contains at least a brief introduction to the topic. Given a point set $Q := \{x_1, \ldots, x_N\} \subseteq \mathbb{R}^n$, the classical Voronoi partition

$$\mathcal{V}_Q := \{V_A \mid A \in \mathcal{P}(Q) \land V_A \neq \emptyset\}, \text{ where } V_A := \left\{y \in \mathbb{R}^n \mid A = \arg\min_{z \in Q} \text{dist}(z, y) \right\}. \quad (5)$$

is a partition of $\mathbb{R}^n$ in the sense of Definition 1 into parts that reflect proximity with respect to the point set $Q$ (see Figure 2a for an illustration in the plane).

Remark 1. The introduction of the Voronoi diagram as a partition and the explicit treatment of lower dimensional elements, e.g. vertices and edges, which are indicated by “multi-valued” images of $\arg\min_{z \in Q} \text{dist}(z, \cdot)$: $\mathbb{R}^n \to \mathcal{P}(Q)$, is not common but crucial, since in the dual partitions to be introduced in Section 3 vertices, edges, and other elements will not be of lower dimension in general and therefore essential to cover the domain of interest.

The key to the definition of the classical Voronoi partition (5) is a map that projects $\mathbb{R}^n$ onto the point set $Q$ (see the definition of $V_A$ in (5)). Since this projection is based on the Euclidean distance, the Voronoi partitions discussed here are often called Euclidean Voronoi partitions. Generalizations with respect to other metrics can be found in [3]. The classical Voronoi partition, as defined in (5), groups those elements of $\mathbb{R}^n$ that are projected onto the same elements of $Q$. In a similar manner Voronoi partitions with respect to a system of closed convex sets $\mathcal{I} = \{I_1, \ldots, I_N\} \subseteq \mathcal{P}(\mathbb{R}^n)$ are introduced. The convex sets $I \in \mathcal{I}$ are denoted as inclusions according to composite material modeling and in contrast to the literature where there sets are typically called generators. We note that the inclusions are not assumed to be pairwise disjoint. They might touch each other. However, general intersections are excluded, i.e. we assume that the intersection of any two inclusions is of lower dimension:

$$\dim(I_1 \cap I_2) \leq \min\{\dim(I_1), \dim(I_2)\}, \quad \dim(I_1 \cap I_2) < \max\{\dim(I_1), \dim(I_2)\} \quad \text{for all } I_1, I_2 \in \mathcal{I}. \quad (6)$$
Condition (6) is fulfilled for all scenarios which are related to touching inclusions, e.g., two cuboids sharing a common boundary face, or triangles sharing exactly a corner.

Convexity and closeness of the elements \( I \in \mathcal{I} \) ensure that the projections onto a single inclusion
\[
\pi_I : \mathbb{R}^n \rightarrow I, \quad x \mapsto \arg\min_{y \in I} \text{dist}(x, y), \quad I \in \mathcal{I},
\]
are well defined. The projection onto the system of sets \( \mathcal{I} \) is given by
\[
\pi_{\mathcal{I}} : \mathbb{R}^n \rightarrow P(\bigcup \mathcal{I}), \quad x \mapsto \arg\min_{y \in \bigcup \mathcal{I}} \text{dist}(x, y) = \arg\min_{y \in \bigcup_{I \subseteq \mathcal{I}} \pi_I(x)} \text{dist}(x, y).
\]
Note that in (7), due to uniqueness, argmin is interpreted as a single-valued function while in (8) the images of argmin are supposed to be finite sets.

The projection \( \pi_{\mathcal{I}} \) induces a mapping \( v_{\mathcal{I}} : \mathbb{R}^n \rightarrow v_{\mathcal{I}}(\mathbb{R}^n) \subseteq P(\mathcal{I}) \) which assigns a subset of inclusions to every point in \( \mathbb{R}^n \):
\[
v_{\mathcal{I}}(x) := \{ I \in \mathcal{I} | \pi_I(x) \cap I \neq \emptyset \}, \quad x \in \mathbb{R}^n.
\]
The map \( v_{\mathcal{I}} \) has a finite image and therefore induces a partition \( \mathcal{V}_{\mathcal{I}} \) of \( \mathbb{R}^n \) denoted as the Voronoi partition with respect to the system of sets \( \mathcal{I} \):
\[
\mathcal{V}_{\mathcal{I}} := \{ V_{\mathcal{A}} | \mathcal{A} \in v_{\mathcal{I}}(\mathbb{R}^n) \}, \quad \text{where } V_{\mathcal{A}} := v_{\mathcal{I}}^{-1}(\mathcal{A}).
\]
We refer to the book [19] for a detailed overview on Voronoi partitions and its generalizations. Especially the case of \( \mathcal{I} \) being a system of discs in \( \mathbb{R}^2 \) (see Figure 2b) and \( \mathcal{I} \) being a system of balls in \( \mathbb{R}^3 \) enjoy great popularity and has been studied in great detail under several names as pointed out in [3, Section 4.5.3].

The remaining part of this section addresses a meaningful classification of the Voronoi elements. The latter classification will be of importance for the definition of generalized Delaunay partitions in the next section. The criterion derived here is not straightforward and requires a closer investigation of set \( v_{\mathcal{I}}(\mathbb{R}^n) \). Remark 2 will show later that obvious classifications such as the dimension of the elements or the cardinality of their corresponding sets of inclusions are not the right choice in general.
By definition there is a one-to-one correspondence between the Voronoi partition \( \mathcal{V}_\mathcal{S} \) and the system of sets \( v_\mathcal{S}(\mathbb{R}^n) \) which gives rise to combinatorial structures. If, for instance, \( \mathcal{S} \) contains only singletons (points in the plane) then \( v_\mathcal{S}(\mathbb{R}^n) \) enriched by \( \emptyset \) forms, up to degenerate situations, an abstract simplicial complex (we refer to Chapter IV in [1] for an overview on complexes and to [9] as well as Chapter 3 in [10] for their applications to mesh generation). Similar results can be derived for general inclusion sets \( \mathcal{S} \). In this article, we are mainly interested in the geometric aspects and want to keep topological aspects as simple as possible. Furthermore, we want to avoid incidences of geometric degeneracy. Therefore we restrict ourselves to the following trivial observation: Since \( v_\mathcal{S}(\mathbb{R}^n) \) is a subset of the power set \( \mathcal{P}(\mathcal{S}) \), the pair \( (v_\mathcal{S}(\mathbb{R}^n), \subseteq) \) is a (finite) partially ordered set (poset), i.e. the subset relation is reflexive, transitive and antisymmetric with respect to \( v_\mathcal{S}(\mathbb{R}^n) \). In connection with the latter observation we briefly remind the reader on basic notations from the theory of ordered sets and refer to the textbook [15] for more exhaustive studies of the topic.

**Definition 2.** Let \((\mathcal{N}, \subseteq)\) be a (finite) poset. The height of an element \( \mathcal{A} \in \mathcal{N} \), denoted by height(\( \mathcal{A} \)), is the greatest non-negative integer \( h \) such that there exists a chain \( \mathcal{B} = \{ \mathcal{A}_0, \mathcal{A}_1, \ldots, \mathcal{A}_h = \mathcal{A} \} \subseteq \mathcal{N} \), where \( \mathcal{A}_0 \subseteq \mathcal{A}_1 \subseteq \cdots \subseteq \mathcal{A}_h \). Accordingly, the height of a system of sets \( \mathcal{N} \), denoted by height(\( \mathcal{N} \)), is given by the maximal height among its elements.

We carry over the notion of height to the elements of the Voronoi partition by simply setting \( \text{height}(V) := \text{height}(v_\mathcal{S}(V)) \) for \( V \in \mathcal{V}_\mathcal{S} \). The attribute height provides the desired classification of Voronoi elements:

\[
\mathcal{V}_\mathcal{S}^h := \{ V \in \mathcal{V}_\mathcal{S} \mid \text{height}(V) = h \}, \quad h = 0, 1, \ldots \text{, height}(\mathcal{V}_\mathcal{S}) \leq n. \tag{11}
\]

We call the elements of \( \mathcal{V}_\mathcal{S}^n \) vertices, the elements of \( \mathcal{V}_\mathcal{S}^{n-1} \) edges, the elements of \( \mathcal{V}_\mathcal{S}^{n-2} \) faces, and so forth. Part (a) of the following remark clarifies that this convention might not coincide with the geometrical imagination of such objects in general.

**Remark 2.**

(a) Voronoi partition (detail). The black shaded area (including the diagonal line) represents the Voronoi ‘edge’ \( v_\mathcal{S}^{-1}(\{I_1, I_2\}) \).

(b) Generalized Delaunay partition. The Delaunay edge \( d_\mathcal{S}^{-1}(\{I_1, I_2\}) \) connecting the generalized vertices \( I_1 \setminus I_2 \) and \( I_2 \setminus I_1 \) is shaded black.

\[ \text{Figure 3: Generalized Voronoi and Delaunay partitions for two intersecting inclusions } I_1 = [0.3, 0.6]^2 \text{ and } I_2 = [0.4, 0.7]^2. \]

**Remark 2.**

a. The height of a Voronoi element does, in general, not correspond to its co-dimension.

Consider, e.g. \( I_1 = B_1(0) \) and \( I_2 = [1, 0]^T \). Then \( \{I_1, I_2\} \in v_\mathcal{S}(\mathbb{R}^2) \) \( v_\mathcal{S}^{-1}(\{I_1, I_2\}) = I_2 \) and \( \text{height}(\{I_1, I_2\}) = 1 \) since \( \{I_1\}, \{I_2\} \in v_\mathcal{S}(\mathbb{R}^2) \). However, \( \dim(v_\mathcal{S}^{-1}(\{I_1, I_2\})) = 0 \). Furthermore, \( v_\mathcal{S}^{-1}(\{I_2\}) = (1, \infty) \times \{0\} \), implying that \( \dim(v_\mathcal{S}^{-1}(\{I_2\})) = 1 \) while \( \text{height}(\{I_2\}) = 0 \).
b. Voronoi elements could also be classified according to the cardinality of their corresponding inclusion sets: $\text{card}(V) := \text{card}(v_\mathcal{S}(V)), V \in \mathcal{Y}_\mathcal{S}$. However, as the dimension, the cardinality of an element does, in general, not coincide with its height; it holds that $\text{height}(V) \leq \text{card}(V) - 1$. The latter inequality can be strict if the combinatorial structure $v_\mathcal{S}(\mathbb{R}^n)$ is not a simplicial complex: Consider, e.g., four points in the plane that are co-circular. Then the intersection of any three corresponding Voronoi elements will be exactly the midpoint of the circumcircle. However, this midpoint (a Voronoi element of height $n = 2$) is only represented as the intersection of all four patches in the combinatorial structure $v_\mathcal{S}(\mathbb{R}^n)$ implying cardinality $4$. If $\text{card}(\mathcal{Y}_\mathcal{S}) := \max_{V \in \mathcal{Y}_\mathcal{S}} \text{card}(V) = \text{height}(\mathcal{Y}_\mathcal{S}) + 1$ then $\text{card}(-)$ and $\text{height}(-)$ coincide on $\mathcal{Y}_\mathcal{S}$.

c. In the classical Voronoi partition $\mathcal{Y}_\mathcal{S}$ defined in (5) the elements are always convex polytopes (see Figure 2a). This property does not carry over to the generalized setting (see Figure 2b). Delaunay elements of height zero can be proved to be star-shaped with respect to their corresponding inclusions but they are not convex, in general. Elements of larger heights might not even be connected as it can be seen from Figure 4a, where a multiply connected Voronoi edge is depicted.

d. The height of the Voronoi partition $\mathcal{Y}_\mathcal{S}$ is limited by $n$ due to assumption (6). We emphasize, that (6) is not a crucial restriction concerning the construction of $\mathcal{Y}_\mathcal{S}$ and the construction of generalized Delaunay partition in Section 3. Consider, e.g., two inclusions $I_1, I_2 \in \mathcal{S}$ having a non-empty intersection of dimension $n$. Then $\{I_1, I_2\} \in v_\mathcal{S}(\mathbb{R}^n)$ and $\text{height}(\{I_1, I_2\}) = 1$ since $\{I_1\}, \{I_2\} \in v_\mathcal{S}(\mathbb{R}^n)$ (see Figure 3a), i.e. $v_\mathcal{S}^{-1}(\{I_1, I_2\})$ is a Voronoi edge of dimension $n$, which shows that new phenomena might appear as soon as (6) is violated.

It is finally important to mention that the generalized Voronoi partitions can be computed efficiently, at least for $\mathcal{S}$ containing circular inclusions in $\mathbb{R}^2$ or spherical inclusions in $\mathbb{R}^3$ [11, 17, 16, 13, 12]. By efficient we mean that the computational complexity is, up to logarithmic factors, proportional to the number of inclusions. A detailed analysis of these algorithms with regard to their applicability to general systems of inclusions is the topic of current research.

3. Generalized Delaunay partitions

The generalized Voronoi partition, introduced in the previous section, and its combinatorial structure can be used to define a generalization of the classical Delaunay triangulation [8]. The latter is a triangulation of a point set $Q \subseteq \mathbb{R}^2$ which is uniquely determined, up to degenerate settings, by Delaunay’s criterion saying
that the circumcircle of any triangle does not contain any elements from \( Q \) apart from its own vertices (see Figure 7a). Several generalizations of this concept are considered in the literature. We emphasize that our construction is different from weighted Delaunay triangulations as they are discussed in [10, Chapter 5] (see also [6, 14]). Furthermore, it is distinct from pseudo triangulations discussed in [23] and from the weighted Delaunay diagram for lines introduced in [18].

We follow the concept of a geometric realization of \( v_\mathcal{I}(\mathbb{R}^n) \) as it is exploited in [9] and in [1, Chapter 4] to derive a generalized Delaunay partition from proximity (Voronoi diagram) with respect to the set of inclusions. For the special case of equally sized circular inclusions, where classical and generalized Voronoi partitions coincide, our resulting partition is equivalent to the one introduced in [5, 4].

Given, as before, a system of closed convex sets \( \mathcal{I} \subseteq \mathbb{P}(\mathbb{R}^n) \) (the inclusions) fulfilling condition (6), we are aiming for a partition \( \mathcal{P}(X_\mathcal{I}) \) of \( X_\mathcal{I} := \text{conv}(\bigcup \mathcal{I}) \) fulfilling \( \mathcal{I} \subseteq \mathcal{P}(X_\mathcal{I}) \). A slightly modified form of the projection \( \pi_\mathcal{I} \) (see (8)) plays a crucial role in its derivation:

\[
\tilde{\pi}_\mathcal{I} : \mathbb{R}^n \rightarrow \mathbb{P}(X_\mathcal{I}), \quad x \mapsto \text{relint} \left( \text{conv} \left( \pi_\mathcal{I}(x) \right) \right).
\] (12)

The image of \( x \in \mathbb{R}^n \) under \( \tilde{\pi}_\mathcal{I} \) is the relative interior of a polytope spanned by the corresponding image of \( x \) under \( \pi_\mathcal{I} \). We will characterize such polytopes more precisely with the help of the following definition.

**Definition 3.**

a. A convex polytope (or polytope for short) \( P = P(x_1, \ldots, x_m), m \in \mathbb{N} \), is the convex hull of the finite point set \( \{x_1, \ldots, x_m\} \subseteq \mathbb{R}^n \). By a strict polytope we denote the relative interior of a polytope. A (strict) polytope \( P = P(x_1, \ldots, x_m) \) is called spherical if there is a hypersphere \( S_P \subseteq \mathbb{R}^n \) such that \( \{x_1, \ldots, x_m\} \subseteq S_P \); \( S_P \) will be denoted as a circumsphere of \( P \), its convex hull \( B_P := \text{conv}(S_P) \) as a circumball of \( P \).

b. Let \( \mathcal{I} \subseteq \mathbb{P}(\mathbb{R}^n) \) be a system of closed, convex sets and let \( \mathcal{A} = \{I_1, \ldots, I_m\} \subseteq \mathcal{I} \), \( m \in \mathbb{N} \). A polytope \( P(x_1, x_2, \ldots, x_m) \) is denoted as a polytope that connects \( \mathcal{A} \) (shortly \( \mathcal{A} \)-connecting) if it is strict, spherical, and fulfills \( x_k \in I_k \) for all \( k = 1, \ldots, m \).

We justify the notion of a strict polytope by the fact that a strict polytope \( P(x_1, \ldots, x_m) \) is the set of all strict convex combinations \( \sum_{i=1}^m \lambda_i x_i \) of its generating elements \( x_1, \ldots, x_m \), where \( \sum_{i=1}^m \lambda_i = 1, \lambda_i \in (0,1) \).
for $i \in \{1, \ldots, m\}$. Note that any polytope spanned by $m \leq n + 1$ elements is spherical. Uniqueness of the circumsphere can be achieved for polytopes with $n + 1$ elements in general position. With regard to Definition 3, the image of $\tilde{\pi}_\mathcal{F}$ contains $\mathcal{A}$-connecting polytopes for certain $\mathcal{A} \subseteq \mathcal{I}$. A key observation is that the polytopes in the image of $\tilde{\pi}_\mathcal{F}$ do not give rise to improper intersections.

**Lemma 1.** For $x, y \in \mathbb{R}^n$ it either holds $\tilde{\pi}_\mathcal{F}(x) = \tilde{\pi}_\mathcal{F}(y)$ or $\tilde{\pi}_\mathcal{F}(x) \cap \tilde{\pi}_\mathcal{F}(y) = \emptyset$.

**Proof.** Let us assume that there exist $x, y \in \mathbb{R}^n$ so that $\tilde{\pi}_\mathcal{F}(x) \cap \tilde{\pi}_\mathcal{F}(y) \neq \emptyset$, $\tilde{\pi}_\mathcal{F}(x) \neq \tilde{\pi}_\mathcal{F}(y)$, and without loss of generality that $\tilde{\pi}_\mathcal{F}(x) \cap \tilde{\pi}_\mathcal{F}(y) \subseteq \tilde{\pi}_\mathcal{F}(x)$ and $\tilde{\pi}_\mathcal{F}(x) \cap \tilde{\pi}_\mathcal{F}(y) \subseteq \tilde{\pi}_\mathcal{F}(y)$ (as contradicting the definition of $\tilde{\pi}_\mathcal{F}$). Then there is a hyperplane $H$ which contains $\tilde{\pi}_\mathcal{F}(x) \cap \tilde{\pi}_\mathcal{F}(y)$ and separates $\tilde{\pi}_\mathcal{F}(x)$ and $\tilde{\pi}_\mathcal{F}(y)$. Therefore $\tilde{\pi}_\mathcal{F}(x) \cap \tilde{\pi}_\mathcal{F}(y) \subseteq \text{bnd}(\tilde{\pi}_\mathcal{F}(x))$, i.e. $z \in \tilde{\pi}_\mathcal{F}(x) \cap \tilde{\pi}_\mathcal{F}(y)$ cannot be written as a strict convex combination of elements of $\tilde{\pi}_\mathcal{F}(x)$ which contradicts our assumption $z \in \tilde{\pi}_\mathcal{F}(x)$. \qed

Lemma 1 remains valid under certain sequential limits as the following corollary states.

**Corollary 1.** Let $(x_k), (y_k) \subseteq \mathbb{R}^n$ be given such that the image sequences $(\tilde{\pi}_\mathcal{F}(x_k)), (\tilde{\pi}_\mathcal{F}(y_k))$ are convergent with respect to the Hausdorff distance. Then it either holds $\lim_{k \to \infty} \tilde{\pi}_\mathcal{F}(x_k) = \lim_{k \to \infty} \tilde{\pi}_\mathcal{F}(y_k)$ or $\lim_{k \to \infty} \tilde{\pi}_\mathcal{F}(x_k) \cap \tilde{\pi}_\mathcal{F}(y_k) = \emptyset$.

In addition to Corollary 1 we show that the closure of the connecting polytopes from the image of $\tilde{\pi}_\mathcal{F}$ indeed covers $X_\mathcal{F}$.

**Lemma 2.** For every $z \in X_\mathcal{F}$ there exists $(x_k) \subseteq \mathbb{R}^n$, so that $z = \lim_{k \to \infty} \tilde{\pi}_\mathcal{F}(x_k)$.

**Proof.** Let $z \in X_\mathcal{F} \setminus (\cup \mathcal{I})$ since otherwise the assertion is proved by choosing $x_k = z$. We pick up the idea of Brown [7] and relate the Delaunay partition to the convex hull of $F_\mathcal{F} := \{(x, f_\mathcal{F}(x)) \in \mathbb{R}^{n+1} \mid x \in \cup \mathcal{I}\}$, where $f_\mathcal{F} : \mathbb{R}^n \to \mathbb{R}, x \mapsto ||x - z||^2$. We interpret every $a \in \mathbb{R}^{n+1}$ as an affine mapping $a : \mathbb{R}^n \to \mathbb{R}, x \mapsto \sum_{i=1}^n a_i x_i + a_{n+1}$. Consider the convex optimization problem

$$\max_{a \in \mathbb{R}^{n+1}} a(z) \quad \text{subject to} \quad a(x) \leq f_\mathcal{F}(x), \forall x \in \cup \mathcal{I}. \quad (13)$$

The admissible set $A := \{a \in \mathbb{R}^{n+1} \mid a(x) \leq f_\mathcal{F}(x), \forall x \in \cup \mathcal{I}\}$ of (13) is closed, convex, and non-empty ($0 \in A$). Thus, (13) admits at least one solution $a^*$. Let $a^*$ be chosen so that the set of points where the inequality constraint is sharp $X := \{x \in \cup \mathcal{I} \mid f_\mathcal{F}(x) = a^*(x)\}$ has minimal cardinality. From the optimality of $a^*$ and the convexity of the inclusions we deduce that $X$ is non-empty and that $z \in \text{relint}(\text{conv}(X))$. Since the function $(f_\mathcal{F} - a^*)(\cdot)$ is quadratic and $\min_{x \in \mathbb{R}^n} (f_\mathcal{F} - a^*)(x) \leq 0$, its zeros lie on a circle $\text{bnd}(B_{r^*}(c^*))$ for some $c^* \in \mathbb{R}^n$ and $r^* \geq 0$. Therefore $X \subseteq \text{bnd}(B_{r^*}(c^*)) \cap (\cup \mathcal{I})$ and $\text{int}(B_{r^*}(c^*)) \cap (\cup \mathcal{I}) = \emptyset$. In fact, $X \subseteq \pi(c^*)$ and there is a sequence $(x_k) \subseteq \mathbb{R}^n$, so that $\lim_{k \to \infty} x_k = c^*$ and $\lim_{k \to \infty} \tilde{\pi}_\mathcal{F}(x_k) = \text{relint}(\text{conv}(X))$. \qed

Following Corollary 1 and Lemma 2, the sequential closure of $\tilde{\pi}_\mathcal{F}(\mathbb{R}^n)$ induces a (possibly infinite) partition of $X_\mathcal{F}$. The generalized Delaunay partition is derived from the latter one by grouping its elements in a suitable manner, i.e. by grouping those elements that are related to the same Voronoi element. This is realized by the mapping $d'_\mathcal{A} : y_\mathcal{A}(\mathbb{R}^n) \to \mathcal{P}(X_\mathcal{F})$, where

$$d'_\mathcal{A} : \mathcal{A} \subseteq y_\mathcal{A}(\mathbb{R}^n) \ni \left\{ \lim_{k \to \infty} \tilde{\pi}_\mathcal{F}(y_k) \right\} | (y_k)_{k \in \mathbb{N}} \subseteq y_\mathcal{A}^{-1}(\mathcal{A}), \tilde{\pi}_\mathcal{F}(y_k) \text{ is convergent} \} \quad \text{for } \mathcal{A} \in y_\mathcal{A}(\mathbb{R}^n). \quad (14)$$
Due to continuity of $\tilde{\pi}_I$ with respect to single Voronoi elements, $d^*_I$ is well defined. The map $d^*_I$ has a finite image since $v_I(\mathbb{R}^n)$ is finite and therefore induces a finite system of subsets $\mathcal{D}_I$ of $X_I$ denoted as the generalized Delaunay partition with respect to the system of sets $\mathcal{I}$:

$$\mathcal{D}_I := \{D_I \mid I \in v_I(\mathbb{R}^n)\}, \quad \text{where } D_I := d^*_I(I).$$

By definition there is a one-to-one correspondence between the elements of $v_I(\mathbb{R}^n)$ and $\mathcal{D}_I$ and consequently between the elements of $\mathcal{V}_I$ and $\mathcal{D}_I$ which is expressed by the mapping $v_I \circ d^*_I$. The following theorem justifies the denotation of $\mathcal{D}_I$ as a partition.

**Theorem 1.** $\mathcal{D}_I$ is a partition of $X_I = \text{conv}(\cup \mathcal{I})$ in the sense of Definition 1.

**Proof.** The assertion is a simple consequence of Corollary 1, Lemma 2, and the fact that $\mathcal{V}_I$ is a partition of $\mathbb{R}^n$. $\square$

As it can be seen from Figure 5b, where a part of a generalized Delaunay partition is illustrated, the elements of $\mathcal{D}_I$ are in general not simplicial, i.e. intervals, triangles, tetrahedrons, etc., but they share certain features with classical triangulations. This will become clearer after applying the notion of height (see Definition 2) to the Delaunay elements: for $D_I = d^*_I(I) \in \mathcal{D}_I$, $I \in v_I(\mathbb{R}^n)$ the height of $D_I$ is defined by $\text{height}(D_I) := \text{height}(I)$. Again, we group the elements according to their height:

$$\mathcal{D}^h := \{D \in \mathcal{D}_I \mid \text{height}(D) = h\}, \quad h = 0,1,\ldots, \text{height}(\mathcal{D}_I) = \text{height}(\mathcal{V}_I) \leq n.$$

Provided the inclusions are pairwise disjoint, the elements of height 0 are exactly the inclusions itself. Otherwise the elements of height 0 are formed by $I \setminus (\cup \mathcal{I} \setminus I) \neq \emptyset$. $I \in \mathcal{I}$. In accordance to classical simplicial subdivisions elements of height 0 are denoted as (generalized) vertices. Elements of $\mathcal{D}^1_I$ share the property that they connect exactly two (generalized) vertices and will therefore be denoted as generalized edges. Further denotation is straight-forward. The elements of largest height $\mathcal{D}^n_I$ are in fact strict spherical polytopes since they are defined via the vertices $\mathcal{V}_I^m$ of the Voronoi partition which are just points. Apart from degenerate situations they are in fact relatively open simplices.
Remark 3.

a. For sets of points in the plane, i.e. $\mathcal{I} = \{\{x_i\} \mid i = 1, \ldots, m\} \subseteq \mathbb{R}^2$, $\mathcal{D}$ coincides with the well-known straight-line dual (see, e.g., [22]) of the Voronoi partition, i.e. the classical Delaunay triangulation, assuming that no four points from $\mathcal{I}$ are co-circular. Sometimes this duality is also referred to as polarity since corresponding edges of $\mathcal{V}_\mathcal{I}$ and $\mathcal{D}_\mathcal{I}$ are orthogonal. In the generalized setting, the orthogonality property generalizes to: For $\mathcal{A} \in \mathcal{V}_\mathcal{I}(\mathbb{R}^n)$ and $\mathbf{z} \in \mathcal{V}^{-1}_\mathcal{I}(\mathcal{A})$ it holds
\[
(\mathbf{x} - \mathbf{y}) \perp T_{\mathcal{V}^{-1}_\mathcal{I}(\mathcal{A})}(\mathbf{z}), \ \forall \mathbf{x}, \mathbf{y} \in \pi_\mathcal{I}(\mathbf{z});
\]
(17)

$b. \mathcal{D}$ is a geometric realization of the combinatorial structure $\mathcal{V}_\mathcal{I}(\mathbb{R}^n)$. It does not preserve the subset relation, but $\mathcal{A} \subseteq \mathcal{B} \in \mathcal{V}_\mathcal{I}(\mathbb{R}^n)$ implies that $\text{cl}(D_{\mathcal{A}}) \cap \text{cl}(D_{\mathcal{B}}) \neq \emptyset$.

c. In general, $\mathcal{A}$ is a height of a Delaunay element and its dimension do not coincide. For instance, $n$-dimensional vertices (inclusions) can be considered and if so, most of the generalized Delaunay edges will have full dimension $n$, as shown in Figure 6.

d. Delaunay elements inherit their connectivity properties from the corresponding Voronoi elements. Therefore, in contrast to the classical setting, connectivity is not guaranteed, e.g., generalized vertices might be connected by a multiply connected edge as it is illustrated in Figure 4b.

Classically, Delaunay triangulations of point sets in general position are uniquely defined by the empty circumcircle criterion mentioned at the beginning of the current section. This criterion is illustrated in Figure 7a. In the remaining part of this section we will introduce a generalized Delaunay criterion and show that the partitions characterized by such a condition indeed are equivalent to (15). In contrast to the classical criterion, the generalized criterion derived here is not only related to the triangles but all to Delaunay elements of any height.

Definition 4. Let $\mathcal{I} \subseteq \mathcal{P}(\mathbb{R}^n)$ be a system of closed, convex sets and let $\mathcal{I} = \{I_1, \ldots, I_m\} \subseteq \mathcal{I}$. An $\mathcal{I}$-connecting polytope $P$ fulfills a generalized Delaunay criterion with respect to $\mathcal{I}$ if it has a circumball $B_P$
that is either a subset of $\cup J$ or a subset of $cl(\mathbb{R}^n \setminus \cup J)$. We shortly denote such a polytope $P$ as a Delaunay polytope.

In addition we will use a notion of maximality. Let $x \in X_J$. An $\mathcal{A}$-connecting Delaunay polytope $P$ which contains $x$ is maximal if there does not exist an $B$-connecting Delaunay polytope which contains $x$ for all $\mathcal{A} \subseteq B \subseteq J$.

The generalized Delaunay criterion suggests the following definition of a map $d_J : X_J \to d_J(X_J) \subseteq \mathbb{P}(J)$:

$$d_J(x) = \mathcal{A} :\iff \text{There exists a maximal } \mathcal{A}-\text{connecting Delaunay polytope } P \text{ which contains } x.$$  \hspace{1cm} (18)

Corollary 1 ensures uniqueness of the polytope $P$ in (18) while existence is due to Lemma 2. Note that $\pi_J$, defined in (12), maps points onto $\mathcal{A}$-connecting Delaunay polytopes.

**Lemma 3.** The mappings $\nu_J$ and $d_J$ induce the same combinatorial structure, i.e. $\nu_J(\mathbb{R}^n) = d_J(X_J)$.

**Proof.** Let $\mathcal{A} \in d_J(X_J)$ be given. Then there exists $x \in X_J$ and a maximal $\mathcal{A}$-connecting Delaunay polytope $P$ that contains $x$, i.e. $P$ has a circumball $B_P$ that is either a subset of $\cup J$ or a subset of $cl(\mathbb{R}^n \setminus \cup J)$. Consider the non-trivial case $B_P \cap (\cup J \setminus \cup \mathcal{A}) = \emptyset$. If further $B_P \cap (\cup J \setminus \cup \mathcal{A}) = \emptyset$ then the center $c$ of $B_P$ is an element of $\nu_J^{-1}(\mathcal{A})$ which implies that $\mathcal{A} \in \nu_J(\mathbb{R}^n)$. If otherwise $B_P \cap (\cup J \setminus \cup \mathcal{A}) \neq \emptyset$ then there is an $\mathcal{A}$-connecting Delaunay polytope $P' = P'(B_P \cap J)$. Due to maximality, $P \subseteq bnd(P')$ and $P \cap P' = \emptyset$ which implies that there is a sequence $(x_k), x_k \to_{k \to \infty} c$, such that $\pi_J(x_k) \to P$. Thus, $\pi_J(x_k) = \mathcal{A}$ for large enough $k$ and $\mathcal{A} \in \nu_J(\mathbb{R}^n)$.

Let conversely $\mathcal{A} = \{I_1, \ldots, I_m\} \in \nu_J(X_J)$ be given. Then there exist $x \in \mathbb{R}^n$ and $\{x_1, \ldots, x_m\}$ such that $x_k \in I_k$ for all $k \in \{1, \ldots, m\}$ and $\pi_J(x) = \{x_1, \ldots, x_m\}$. In fact $\pi_J(x)$ spans a maximal $\mathcal{A}$-connecting Delaunay polytope which implies that $\mathcal{A} \in d_J(X_J)$.

Lemma 3 states that if a set of inclusions is connected by a Delaunay element then it is also connected by an element of the partition that is induced by the preimage of $d_J$ and vice versa. In fact, the connecting elements are equal in the geometric sense.

**Theorem 2.** It holds that $\mathcal{D}_J = \{d_J^{-1}(\mathcal{A}) \mid \mathcal{A} \in d_J(X_J)\}$, i.e. the generalized Delaunay partition is induced by $d_J$.

**Proof.** Given $\mathcal{A} \in \nu_J(\mathbb{R}^n)$, we will show that $d_J^+ \mathcal{A} = d_J^{-1}(\mathcal{A})$. Let $x \in d_J^+ \mathcal{A}$. Then there is a convergent sequence $(y_k) \subseteq \nu_J^{-1}(\mathcal{A})$ so that $x \in \lim_{k \to \infty} \pi_J(y_k)$ which implies that $x \in d_J^{-1}(\mathcal{A})$ since $\lim_{k \to \infty} \pi_J(y_k)$ is a maximal $\mathcal{A}$-connecting Delaunay polytope that contains $x$.

Let conversely $x \in d_J^{-1}(\mathcal{A})$, then there is a maximal $\mathcal{A}$-connecting Delaunay polytope $P$ that contains $x$. Following the first part of the proof of Lemma 3 $P = \pi_J(e)$, where $e$ is the midpoint of a circumball of $P$, or there is a sequence $(x_k) \subseteq \nu_J^{-1}(\mathcal{A})$ such that $x_k \to_{k \to \infty} e$ and $\pi_J(x_k) \to P$. Both cases imply that $P \subseteq d_J^+ \mathcal{A}$ and therefore $x \in d_J^+ \mathcal{A}$.

For the purpose of further illustrating the discussion we give two more examples of generalized Delaunay partitions. In Figure 8 the generalized Delaunay partition with respect to a set of squares in the plane is visualized to make clear that there are no smoothness restrictions to the inclusions. In Figure 10 the generalized Delaunay partition with respect to a set of balls in space is depicted to emphasize that generalized Delaunay partitions are not limited to the 2-dimensional setting.
Remark 4. Generalized Delaunay partitions can be computed easily from their Voronoi counterparts as indicated in Remark 3(a). We have already given references to fast algorithms (almost $O(\text{card}(\mathcal{F}))$) for computing generalized Voronoi partitions at the end of the previous section (see page 7) for the special case of circular/spherical inclusions. Algorithmic aspects of generalized Delaunay partitions for general (convex) inclusion sets are a topic of current research.

To indicate the simple usage of generalized Delaunay partitions we want to explain its construction from its Voronoi counterpart in a model situation. Moreover, a suitable parametrization of its elements (edges) is given to show that these partitions can be used easily within finite element methods.

Example 1. Consider pairwise distinct circular inclusions $\mathcal{I}$ and let $\mathcal{V}_\mathcal{I}$ and $\mathcal{D}_\mathcal{I}$ denote the corresponding Voronoi and Delaunay partitions. Let $E_V \in \mathcal{V}_\mathcal{I}$ denote the Voronoi edge separating two inclusions $I_1, I_2$. By $E_D$ we denote the corresponding Delaunay edge connecting the two inclusions $I_1, I_2$. Without loss of generality we assume that $I_1 = B_{r_1}(x^1)$ and $I_2 = B_{r_2}(x^2)$, where $r_1, r_2 \geq 0, x^1 = 0, x^2 = [0, \delta]^T, \delta > r_1 + r_2$. Assuming connectedness of $E_V$ and $E_D$, respectively, there exist $-\frac{\pi}{2} \leq \alpha \leq \beta \leq \frac{\pi}{2}$ in such a way that

\[
\pi_1(E_V) = (r_1 \sin([\alpha, \beta]), r_1 \cos([\alpha, \beta]))^T \quad \text{and} \\
\pi_2(E_V) = (r_2 \sin([\alpha, \beta]), \delta - r_2 \cos([\alpha, \beta]))^T. 
\]

The parameters $\alpha$ and $\beta$ can be computed easily by simply projecting the Voronoi vertices which bound $E_V$ onto one of the inclusions. As indicated in Remark 3(a) a parametrization of $E_D$ can be given by the (diffeomorphic) mapping $J_{E_D} : [\alpha, \beta] \times [0, 1] \rightarrow \text{int}(E_D)$

\[
J_{E_D}(s, \lambda) = \left( \begin{array}{c} ((1 - \lambda)r_1 + \lambda r_2) \sin(s) \\ ((1 - \lambda)r_1 - \lambda r_2) \cos(s) + \delta \lambda \end{array} \right). \tag{19} 
\]

The mapping is visualized in Figure 9. Note that the generalized edge $E_D$ is uniquely determined by the inclusion data and the values of $\alpha, \beta, \text{and } \delta$. 

Figure 8: Generalized Delaunay partition with respect to squares in the plane.
Finally, we want to mention that the generalized Delaunay partitions can also be derived as the limit of classical Delaunay partitions with respect to a convergent sequence of polygonal approximations of the inclusions. We refer to [20] for an intuitive description of this procedure.

**Conclusion and future work.** We have introduced a new concept for partitioning domains with respect to a given system of subdomains. Driven by applications from composite material modeling we have thereby generalized the concept of a Delaunay partition. A generalized concept of duality with respect to Voronoi tessellations has been derived. The paper provides the basis for finite element computations on composite materials as well as other problems where the meshes need to match certain geometric details of the problem. Currently, in [21], generalized Delaunay partitions are employed within finite element computations the heat conductivity problem (1). Generalized Delaunay partitions can also be used to define structural (network) approximations to the conductivity problem as indicated in [5, 4]. Furthermore, these partitions provide a conforming mesh which is helpful within composite quadrature formulas on complicated domains.

The main advantage of generalized Delaunay partitions is its minimality with respect to the problem data. Its elements are simple geometric objects compared to the geometry of the inclusions. The focus in this article was clearly on the conceptual development of generalized Delaunay partitions. Algorithms and its complexity analysis are not given in the general setting but references to existing literature in special cases are given (see Remark 4). The derivation of fast algorithms for general (convex) inclusions is a task of future research. To the same degree, non-convex inclusions have to be considered to successfully bridge the gap to a wide range of practical applications.
References