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Anomalies in quasi-triangulations and beta-complexes of spherical atoms in molecules

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ABSTRACT

The beta-complex is the most compact and efficient representation of molecular structure as it stores the precise proximity among spherical atoms in molecules. Thus, the beta-complex is a powerful tool for solving otherwise difficult shape-related problems in molecular biology. However, to use the beta-complex properly, it is necessary to correctly understand the anomalies of both the quasi-triangulation and the beta-complex. In this paper, we present the details of the anomaly of the beta-complex in relation to the quasi-triangulation. With a proper understanding of anomaly theory, seemingly complicated application problems related to the geometry and topology among spherical balls can be correctly and efficiently solved in rather straightforward computational procedures. We present the theory with examples in both $\mathbb{R}^2$ and $\mathbb{R}^3$.

1. Introduction

The quasi-triangulation is the dual of the Voronoi diagram of spherical balls, and thus they have identical information on the proximity among the balls. The beta-complex is a subset of the quasi-triangulation and represents the precise proximity among the balls within and on the boundary of a set of balls where the boundary is defined with respect to a spherical probe that accesses the ball set. The beta-complex can be efficiently computed from the quasi-triangulation. For the details of the Voronoi diagram of balls, the quasi-triangulation, and the beta-complex, see [1–4].

The beta-complex has proven its powerful capability in reasoning the spatial structure among a set of atoms in a molecule and many important applications in computational and structural molecular biology have been found. Applied to the problems in molecular biology, the beta-complex is a powerful computational tool for correctly and efficiently solving otherwise difficult shape- and/or geometry-related problems due to its dual properties stated as follows:

- *Precise Proximity*. The beta-complex has precise proximity information among all atoms both within and on the boundary of a molecule where the boundary is defined by a probe.
- *Concise Abstraction*. The beta-complex only has the topology information of the nearest neighbors for each atom in the form of the connectivity among its simplexes.

Additionally, the beta-complex has the following property:

- *Multi-resolution*. The beta-complex can be defined with respect to the probe of a desired radius.

The Protein Data Bank (PDB) files [5–7], for example, contain a precise molecular representation but do not have any proximity information. Examples of using the "precise proximity" perspective include the computation of the Connolly surface of a molecule [8,9] and the computation of molecular mass properties such as the van der Waals volume and the van der Waals area [10]. Examples of using the "concise abstraction" perspective include the recognition of a potential binding site, called a pocket, of a compound on a molecular boundary [11] and a fast docking simulation [12]. All these problems, including many more to be found, can be efficiently solved using the single framework of the quasi-triangulation and beta-complex.

However, to use the quasi-triangulation and the beta-complex properly, it is necessary to understand them correctly. Despite its usefulness, the beta-complex may seem at first somewhat

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difficult to understand because it is in general not necessarily a simplicial complex. From the interactions with users of the beta-complex, we have learned that the notion of *anomaly* is the core part of the difficulty because it is a new concept that the simplicial complex does not possess. In order to use the beta-complex properly, it is necessary to correctly understand the anomalies in the beta-complex. The Delaunay and the regular triangulations, which are respectively the duals of the ordinary Voronoi diagram of points and the power diagram, are simplicial complexes whose mathematical and computational properties are simple, powerful, and well-known [13–15]. However, the quasi-triangulation is not necessarily a simplicial complex and its mathematical and computational properties are currently actively being studied and reported. The topological properties that cause the quasi-triangulation to violate the conditions of a simplicial complex is termed as an "anomaly". It turns out that there are very few well-defined anomaly cases in both $\mathbb{R}^2$ and $\mathbb{R}^3$.

Given a set of disks in $\mathbb{R}^2$ and a set of spheres in $\mathbb{R}^3$ with different radii, the quasi-triangulation may be either simplicial or non-simplicial depending on the configuration of the input spheres. If the quasi-triangulation is simplicial, the beta-complex is also simplicial and its application to shape-related problems is obvious. When the quasi-triangulation is non-simplicial, the beta-complex can be either simplicial or non-simplicial depending on the probe size that is usually denoted by the parameter β. If the quasi-triangulation is non-simplicial but the beta-complex is simplicial, the use of the beta-complex is still straightforward. However, if both the quasi-triangulation and the beta-complex are non-simplicial, a conceptual difficulty may arise for properly using the beta-complex which may seem counter-intuitive.

This paper presents the anomalies of the quasi-triangulation and the beta-complex in $\mathbb{R}^2$ and $\mathbb{R}^3$ and shows that the not-yet-familiar concept of anomaly can be easily explained and used correctly. With the proper understanding of the anomaly theory, complicated geometry problems among spherical particles can be correctly and efficiently solved in a rather straightforward computational procedure. We present the theory of anomaly using the problem to compute the volume of the region of the space taken by the union of three-dimensional spherical atoms constituting a molecule. This is because researchers in molecular biology are frequently interested in calculating various types of molecular properties and it turns out that many of these properties are functions of the volume (and/or the area) of the region of space taken by a molecule or its offset. To aid reader comprehension, we first present an anomaly in $\mathbb{R}^2$ with the problem to compute the area of the region in the plane taken by the union of circular disks in the plane.

Section 2 introduces some preliminary computational building blocks with their definitions and properties. Section 3 presents the basic concept of an anomaly in the quasi-triangulation of circular disks in $\mathbb{R}^2$. Section 4 presents the relationship between the anomaly of the quasi-triangulation and the anomaly of the beta-complex of three disks in the plane. Section 5 presents a similar phenomenon for five disks. Section 6 presents an anomaly for spherical balls in $\mathbb{R}^3$. Section 7 concludes the paper.

2. Preliminaries

Let $A = \{a_1, a_2, \ldots, a_n\}$ be a set of three-dimensional spherical atoms where $a_i = (c_i, r_i)$ denotes an atom with the center c_i and radius $r_i \geq 0$. The Voronoi diagram $\mathcal{VD}$ of A is the tessellation of the space where each location in the space is assigned to the boundary of the closest atom $a \in A$ where the distance is defined by the ordinary Euclidean distance. Note that $\mathcal{VD}$ is different from the ordinary Voronoi diagram of points. For the details of $\mathcal{VD}$, see [1,16–18]. Given $\mathcal{VD}$, its dual structure called the quasi-triangulation $\mathcal{QT}$ is defined by dual mapping: from a vertex in $\mathcal{VD}$ to a tetrahedral cell in $\mathcal{QT}$, from an edge in $\mathcal{VD}$ to a triangular face in $\mathcal{QT}$, from a face in $\mathcal{VD}$ to an edge in $\mathcal{QT}$, and from a cell in $\mathcal{VD}$ to a vertex in $\mathcal{QT}$ where the vertex coincides with the center of a related atom. The quasi-triangulation $\mathcal{QT}$ can be represented as a quadruplet $\mathcal{QT} = (V^Q, E^Q, F^Q, C^Q)$ where V^Q, E^Q, F^Q, and C^Q are the sets of vertices, edges, faces, and cells in the quasi-triangulation, respectively. In this paper, for notational simplicity, we denote the vertex set as $V^Q = \{a_1^Q, a_2^Q, \ldots, a_n^Q\}$ where a vertex $a_i^Q \in V^Q$ corresponds to the center of the corresponding atom a_i^Q. Similarly, $e_{ij} \in E^Q$ denotes that the edge is defined by the vertices a_i^Q and a_j^Q (to be specific, the centers of a_i^Q and a_j^Q), $f_{ijk} \in F^Q$ denotes that the face is defined by the vertices a_i^Q, a_j^Q, and a_k^Q, and $c_{ijkl} \in C^Q$ denotes that the cell is defined by the vertices a_i^Q, a_j^Q, a_k^Q, and a_l^Q, all these simplexes with the orientation given by the order of the indices. The conversion between $\mathcal{VD}$ and $\mathcal{QT}$ can be done in linear time with respect to the number simplexes in $\mathcal{QT}$. It is assumed in this paper that the topologies of $\mathcal{VD}$ and $\mathcal{QT}$ are stored in an appropriate data structure such as the radial-edge data structure [19] and the inter-world data structure [4], respectively. It is important to note that two d-dimensional simplexes in $\mathcal{QT}$ can be in contact at more than one $(d-1)$-dimensional simplex. Hence, $\mathcal{QT}$ is not necessarily a simplicial complex. For the definition of a simplicial complex, see [15,20,21]. For the details of $\mathcal{QT}$, see [3,4].

Two cells in $\mathcal{QT}$ are called *face-connected* if they share a face. If two cells share k faces, they are said to be *k-connected*. Two cells in the simplicial complex are 1-connected, if they are face-connected. However, two cells in $\mathcal{QT}$ in $\mathbb{R}^3$ are not necessarily 1-connected, but they may be 2-, 3-, or 4-connected. Hence, $\mathcal{QT}$ is not necessarily a simplicial complex. In $\mathbb{R}^3$, the face-connected cells in $\mathcal{QT}$ form a cluster of cells called a *world* and there can be more than one world in a $\mathcal{QT}$. In other words, in theory, there can be more than one world where each world is disconnected from other worlds from the face-connectivity point of view. Hence, there can be a hierarchy among worlds in the quasi-triangulation in that one world may contain another. A world containing another is called a *big-world* and one contained in another is called a *small-world*. In this sense, "big" and "small" are relative terms. The containment of worlds may repeat in that a small-world may contain a smaller world, and a smaller world may also contain an even smaller world, and so on. The biggest world is called the *root-world* and there is only one root-world in $\mathcal{QT}$. The k-connectedness (where $k = 2, 3$, and 4 in $\mathbb{R}^3$) and the world hierarchy makes $\mathcal{QT}$ a non-simplicial complex and these conditions are called *anomalies* in the quasi-triangulation. For details, see [2–4].

Each simplex $\sigma \in \mathcal{QT}$ is associated with four *bounding states*: *exterior*, *singular*, *regular*, and *interior*. A simplex σ is called singular if it does not bound any higher-dimensional simplex and regular if it bounds some higher-dimensional simplex. All the singular and regular simplexes constitute a network of simplexes denoted by the symbol $\partial\mathcal{S}_\beta$. A simplex σ is called interior or exterior if it is interior or exterior to $\partial\mathcal{S}_\beta$, respectively. If a real-valued parameter β (which is the radius of a spherical probe) is given, σ is assigned by one of the four bounding states where its interpretation is as follows: if σ is singular, the atom(s) corresponding to the vertex(es) of σ can be touched by the probe from more than one direction; if σ is regular, its corresponding atom(s) can be touched by the probe from only one direction; if σ is interior, its corresponding atom(s) cannot be touched by the probe from any direction due to another atom's hindrance; otherwise, σ is exterior and its corresponding atom(s) cannot be touched simultaneously by the probe from any direction because the probe size is not big enough. A vertex cannot be exterior independent of its dimension.