ERC Advanced Grant 2017
Research Proposal [Part B1]

Alpha Shape Theory Extended

Alpha

Name of the Principle Investigator (PI):	Herbert Edelsbrunner,
Name of the PI's host institution for the project:	IST Austria,
Proposal duration in months:	60.

Proposal Summary

Alpha shapes were invented in the early 80s of last century [18], and their implementation in three dimensions in the early 90s [20] was at the forefront of the exact arithmetic paradigm [33] that enabled fast and correct geometric software. In the late 90s, alpha shapes motivated the development of the wrap algorithm for surface reconstruction [14], and of persistent homology [19], which was the starting point of rapidly expanding interest in topological algorithms aimed at data analysis questions [6, 16]. We now see *alpha shapes*, *wrap complexes*, and *persistent homology* as three aspects of a larger theory, which we propose to fully develop. This viewpoint was a long time coming and finds its clear expression within a generalized version of discrete Morse theory [23]. This unified framework offers new opportunities, including

(I) the adaptive reconstruction of shapes driven by the cavity structure;

(II) the stochastic analysis of all aspects of the theory;

(III) the computation of persistence of dense data, both in scale and in depth;

(IV) the study of long-range order in periodic and near-periodic point configurations.

These capabilities will significantly deepen as well as widen the theory and enable new applications in the sciences. To gain focus, we concentrate on low-dimensional applications in structural molecular biology and particle systems.

Section a: Extended Synopsis of the Scientific Proposal

We review the technical components on which this proposal is based, mention some of their extensions, discuss algorithms, and finally list applications we address.

A. FUNDAMENTAL INGREDIENTS

Our study combines geometric, topological, and algebraic ingredients to a powerful theory that facilitates inroads into a number of applied fields. These applications warrant detailed investigations and motivate the computational and mathematical developments. We begin with brief introductions of the three main ingredients: alpha shapes, wrap complexes, and persistent homology.

Alpha shapes. Let X be a finite set of points in d-dimensional Euclidean space, $\mathbb{R}^d$, and let $r \geq 0$. The most direct definition of the alpha shape starts with the *Voronoi tessellation* of X and its dual *Delaunay mosaic*, which we denote as $\mathrm{Del}(X)$; see [15] and the left panel of Figure 1. Write X_r for the set of points at distance at most r from at least one data point, and note that the Voronoi tessellation decomposes X_r into convex sets, each the intersection of a round ball with a convex polyhedron. Taking the dual of this decomposition, we get the *alpha complex* for radius r, denoted $\mathrm{Alpha}_r(X)$, which we observe is a subcomplex of the Delaunay mosaic; see the right panel of Figure 1. The *alpha shape* for radius r is the part of $\mathbb{R}^d$ covered by the simplices of $\mathrm{Alpha}_r(X)$. For simplicity and without loss of generality, we

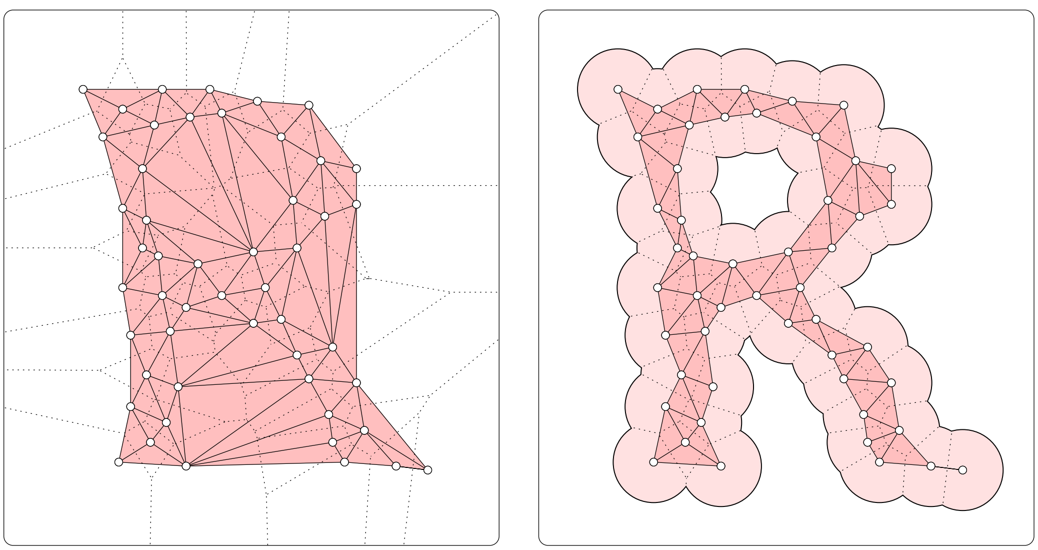

Figure 1: *Left:* a Voronoi tessellation in the plane (dotted) and its dual Delaunay mosaic (solid and shaded) superimposed. Only the Voronoi edges within the rectangular window and their dual Delaunay edges are shown. *Right:* the Voronoi decomposition of the union of balls centered at the data points and the dual alpha complex superimposed.

assume that X satisfies a suitable general position requirement so that the Delaunay mosaic is a simplicial complex. It follows that $\mathrm{Alpha}_r(X)$ is a simplicial complex for every r.

When r increases, $\mathrm{Alpha}_r(X)$ stays constant or gains new simplices. It follows that for each simplex there is a threshold beyond which the simplex belongs to the alpha complex. Write $f\colon \mathrm{Del}(X) \to \mathbb{R}$ for the function that maps each simplex to this threshold, refer to f as the *radius function* on the Delaunay mosaic, and observe that the alpha complexes are its *sublevel sets*: $\mathrm{Alpha}_r(X) = f^{-1}[0, r]$ for every $0 \leq r \leq \infty$.

Wrap complexes. The original paper on this topic was written in terms of smooth approximations of a piecewise linear function [14]. Here we use the language of discrete Morse theory [23, 24], which allows for a compact definition based on the radius function on the Delaunay mosaic. Ordering the sublevel sets from smallest to largest, we suppose that r_i is the smallest real number such that $K_i = f^{-1}[0, r_i]$ is the i-th alpha complex. The difference to the preceding alpha complex, $K_i \setminus K_{i-1}$, consists of all simplices in the Delaunay mosaic whose smallest empty circumscribed sphere has radius r_i. Assuming general position, these simplices form an *interval* in $\mathrm{Del}(X)$; that is: there are simplices $P, R \in \mathrm{Del}(X)$, with $P \subseteq R$, such that the interval is $[P, R] = \{Q \in \mathrm{Del}(X) \mid P \subseteq Q \subseteq R\}$. In other words, the radius function partitions the Delaunay mosaic into intervals, and we distinguish between *singular intervals*, defined by $P = R$, and *non-singular intervals*, for which P is a proper face of R. The *critical simplices* of f are the ones that belong to singular intervals.

The partition into intervals provides extra structure, which we exploit to define the *wrap complex* for radius r, denoted $\mathrm{Wrap}_r(X)$, as the complex obtained from $\mathrm{Alpha}_r(X)$ by collapsing all non-singular intervals that can be collapsed. To explain what this means, let $[P, R]$ be a non-singular interval whose simplices belong to $\mathrm{Alpha}_r(X)$. If P is not a face of any simplex outside its interval, we can remove all simplices of the interval from the alpha complex, an operation we refer to as a *collapse*. Iterating this step, we eventually get $\mathrm{Wrap}_r(X)$. Indeed, it is not difficult to prove that the set of removed simplices does not depend on the sequence in which we collapse the intervals. A collapse preserves the homotopy type, which implies that $\mathrm{Wrap}_r(X) \subseteq \mathrm{Alpha}_r(X)$ have the same homotopy type and therefore isomorphic homology groups. Historically, the main reason for introducing wrap complexes was for surface reconstruction [11, 14], and we add Objective (I) as another motivation to study and further develop the concept.

Persistent homology. Using the radius function on the Delaunay mosaic, we get a *filtration* of alpha complexes: $\emptyset = K_0 \subseteq K_1 \subseteq \ldots \subseteq K_n = K$. As mentioned earlier, the difference between contiguous complexes is either a critical simplex or a non-singular interval of simplices. The two complexes have non-isomorphic homology groups in the former case and isomorphic homology groups in the latter case. More precisely, upon adding a critical p-simplex, either the p-th homology group gains a generator or the $(p-1)$-st homology group loses a generator. We call the first event a *birth* and the second event a *death*. The main insight of persistence is that there is a canonical pairing between the births and the deaths that encodes a rich amount of information about the complexes in the filtration, richer than just the ranks of their homology groups. A more elaborate introduction of persistent homology will be given in the main body of the proposal, but see also [7, 16, 19, 25]. Here we are content with an elementary discussion of the extra information contained in the birth-death pairs.

Suppose a p-simplex gives birth to a generator of the p-th homology group, and later in the filtration a $(p+1)$-simplex gives death to this generator. In $\mathbb{R}^3$, we have such events for $p = 0, 1, 2$. The case $p = 0$ is special because all vertices are born simultaneously, at $r = 0$, and we count as many gaps as there are vertices minus 1. A gap dies when an edge connects the two components it separates. This is just like in hierarchical clustering, but there are two more interesting cases. For $p = 1$, we witness the birth of a *tunnel* when an edge completes a loop, and its death when the last in a series of triangles closes the tunnel. For $p = 2$, we witness the birth of a *void* when a triangle completes the enclosing surface, and its death when the last in a series of tetrahedra fills the void. For each $i \leq j$, we have a *persistent homology group*, which counts the homology classes born before or at K_i and dying at K_j or later. We represent the pairing combinatorially as a multiset of points in the extended plane, drawing the time of birth horizontally and the time of death vertically. Calling this multiset the *persistence diagram* of the filtration, we can see the ranks of the homology groups as the numbers of points in upper-left quadrants anchored on the diagonal. The extra information are the ranks of the persistent homology groups, which we can see as the numbers of points in upper-left quadrants anchored *above* the diagonal.

B. EXTENSIONS

The main concepts of our theory have far-reaching extensions, of which we list the four that are most relevant to applications pursued in this project.

To deal with spheres of different sizes, we generalize the Voronoi tessellation and Delaunay mosaic to **weighted points**, $X \subseteq \mathbb{R}^d \times \mathbb{R}$. The *weighted squared distance* of an unweighted point $a \in \mathbb{R}^d$ from a weighted point $(x, w_x) \in X$ is $\|a - x\|^2 - w_x$. Retracing the definition of the Voronoi tessellation for unweighted points with this notion of distance, we get the *weighted Voronoi tessellation* and the *weighted Delaunay mosaic* of X [1], but also the *weighted alpha shape* and the *weighted wrap complex* of X for a radius r [13].

Assuming **dense data** in the form of a discrete set $X \subseteq \mathbb{R}^d$, we choose a positive integer k, and we decompose space based on the k closest points in X. Specifically, the domains in the *order-k Voronoi tessellation* of X are maximal subsets of $\mathbb{R}^d$ such that any two points in a subset have the same k closest points in X, with ties ignored [30]. The *order-k Delaunay mosaic* is easy to define abstractly, as the dual of the order-k Voronoi tessellation, and there is a natural geometric realization obtained by mapping every domain to the average of its k closest points, which is a point in $\mathbb{R}^d$ [2]. Given a radius $r \geq 0$, we can restrict the construction of the order-k Voronoi tessellation to the *k-fold cover*, which consists of all $a \in \mathbb{R}^d$ whose k closest points are within distance r from a. This leads to the definition of the *order-k alpha shape* of X for r, which captures the homotopy type of the k-fold cover [17].

Letting $X \subseteq \mathbb{R}^d$ be discrete, the **k-th Brillouin zone** of $x \in X$ is the set of points $a \in \mathbb{R}^d$ for which x is the k-th closest point of X, with ties ignored. Note the connection to the order-k Voronoi tessellation of X. These zones have originally been introduced in crystallography [5] and have been used to study lattices, which are sets X that are periodic in d linearly independent directions. For example, it is known that for every x and k, the d-dimensional volume of the k-th Brillouin zone centered at x is the determinant of the matrix of basis vectors spanning the lattice [4].

A **vineyard** is a time-series of persistence diagrams [10]. Imagine, for example, a slowly folding protein. At any moment in time, $t \in [0, 1]$, the data is a collection of (possibly weighted) points in $\mathbb{R}^3$, each the center of an atom of the protein. Correspondingly, we get a persistence diagram, which provides a multi-scale description of the shape at time t. Running the process from beginning to end, we get a 1-parameter family of persistence diagrams. As proved in [9], the transformation to the persistence diagram is 1-Lipschitz, which implies that each point in the diagram changes continuously with time. Stacking up the persistence diagrams of the 1-parameter family, we see each point move along a connected path, which we call a *vine*. The collection of vines is the *vineyard* of the folding protein.

C. ALGORITHMS

There are fast algorithms and also publically available software for many but not all concepts in our theory. We briefly discuss the current state and mention where improvements of algorithms and software are needed and where new algorithms and software is desired.

There are fast algorithms for constructing **Voronoi tessellations and Delaunay mosaics**, both with floating-point and with exact arithmetic, and we mention CGAL — the computational geometry algorithms library — as a popular source for both. We prefer exact arithmetic because small errors can get large by propagation and lead to unexpected events. In two and three dimensions, this software is fast because well optimized, but in four and higher dimensions we desire faster code for the time in the future when applications that go beyond the usual three dimensions will have matured. There is little difference between the algorithms in the weighted and the unweighted cases. Order-k Delaunay mosaics can be constructed as weighted order-1 Delaunay mosaics. The naive way to do this computes a weighted point for every subset of size k, but many will be redundant, which slows down the algorithm. A better option is the incremental algorithm, which computes the order-k from the order-$(k-1)$ Delaunay mosaic, and we have developed a version that is simple enough to have an effective implementation as part of Objective (III).

Given a weighted or unweighted Delaunay mosaic, the computation of the **radius function** is straightforward but not without pitfalls. Even here, floating-point arithmetic can lead to fatal errors, for example when the computed radii violate the interval structure or, worse, give rise to sublevel sets that are not subcomplexes of the mosaic. These structural constraints need to be kept in mind, and they need to be corrected for in cases in which the radius function is computed only approximately. Given a radius function on a weighted or unweighted Delaunay mosaic, it is easy to construct an **alpha complex** by selecting simplices, and a **wrap complex** by further collapsing non-singular intervals. There are however still open questions about the efficient computation of modifications of the wrap complex, eg. for the adaptive reconstruction of shapes mentioned as Objective (I) in the Proposal Summary.

While **persistent homology** is the youngest of the main ingredients of the theory, its algorithms have received much attention within the context of topological data analysis and enjoyed a rapid development to ever faster and widely available software, including JAVAPLEX [32], DIONYSUS [29], and PHAT [3]. Nonetheless, there is room for improvement but also for expansion. For example, most algorithms assume that the linear maps between the homology groups are induced by inclusions between the complexes in the filtration. Recently, algorithms for simplicial maps between the complexes have been considered [12]. However, the linear maps we encounter in our approach to Objective (III) are more general yet. Even when the linear maps are induced by inclusions, there are questions that are currently unanswered. Some relate to the exhaustive reduction algorithm for persistence, which we use to approach Objective (I) [19]. It tends to lead to less sparse matrices than the traditional algorithms, but the extra information is useful, as we will see.

Another direction with room for improvement concerns algorithms and software that compute **vineyards**, for which the only widely available software we are aware of assumes a fixed mosaic [29]. For applications to dynamic molecules, we need a vineyard algorithm that is customized for Delaunay mosaics defined by moving points in $\mathbb{R}^3$, and we desire an extension to two or more independent time-parameters.

D. CONNECTIONS TO APPLICATIONS

We derive the motivation for the development of the geometric concepts and their algorithms from applications. Because of the wide range of possibilities, we need to make choices to prevent becoming unfocused, and we favor low-dimensional questions that have to do with molecules and with materials. We describe four such connections, briefly sketching the background and the connections to our objectives.

Transport pathways and adaptive reconstruction. The interaction between biomolecules takes place in *cavities*, which loosely speaking are surface depressions and protrusions of matching size and shape. A particularly interesting such interaction passes a signal from one side of a cell membrane to the other. This may happen through allostery, which is a concerted adjustment of the conformation that propagates a change in shape, or by channeling a particle through the membrane. We refer to [8] for software supporting the search for such transport pathways.

The functional channel in a protein is often the most persistent tunnel in the corresponding alpha shape filtration. It is therefore desirable to reconstruct the shape with precisely this one tunnel, but chances are that there is not a single alpha shape with this property. In this case, there is also not a single wrap complex with this property, but we can use the interval structure of the radius function to force the property in the reconstruction. In the main body of this proposal, we will give details on how to combine the wrap algorithm with an embellished version of persistent homology that provides information about dependences between the holes, which we need to take into account since we desire some tunnels but not others in the reconstructed shape. Other than through tunnels in 3D shapes, a particle can also be transported inside a bubble that moves through a shape in time. Such transport is difficult to observe experimentally so that searching for 1-dimensional pathways through 4D shapes will enter unchartered land both in theory and in practice. We combine our technology to trace and reconstruct holes with parametrized representations of shape (vineyards) to support the search for such elusive transport pathways.

Shape classification and stochastic geometry. The desire to build databases of shapes arises in many contexts, for example of materials, for which it is essential to capture the hole structure within [27]. In structural molecular biology, proteins and other biomolecules have elaborate classification schemes, but these are often not or not only based on shape. A class of proteins for which a classification based on geometric shape is desirable arises in the study of viruses. While many of these proteins have little sequence similarity, they can substitute for each other in the assembly of the capsid, and the viruses switch between them under environmental pressure [31].

We suggest to use the space of persistent diagrams as the mathematical basis of a shape database for these proteins. While this idea is not new, its details are not well understood. We contribute with stochastic studies of random data to provide a baseline for comparison. Building on recent analytic results for Poisson point processes [22, 21], we gather experimental data (and get analytic expressions where possible) for persistence diagrams of the Delaunay radius function and for birth-giving versus death-giving simplices in the corresponding filtration.

Dense data and multiple covers. The topological aspects of data analysis are about the shape of data, but often this means the shape of the bulk, or the region where the data exceeds a density threshold. Such restrictions may be motivated by statistical considerations or the need to cope with too much data.

We approach dense data by studying the k-fold cover for a non-negative radius, r, which is the subset of space within distance at most r from at least k data points. The order-k Voronoi tessellation decomposes this cover into convex pieces, giving a filtration of order-k alpha complexes that have the same persistence diagram as the k-fold covers. While there are no major mathematical obstacles, there are computational challenges that we had to overcome to develop fast software for the tessellations and the persistence diagrams. In contrast, fixing r and varying k leads to a more interesting but also more challenging task. The main obstacle to developing an algorithm is the fact that the alpha complexes for different depth values are not in any obvious way related to each other. We will explain ideas how to overcome this difficulty in the main body of this proposal.

Near-periodic systems and long-range order. With some idealization, the atoms in metals but also other materials are arranged in 3-dimensional lattices. In reality however, metals form chunks of lattices, called *grains*, with violations of the global order where neighboring grains meet along surfaces and junctions [28]. Another deviation from global order is a relaxation throughout the material, as observed for example in glass [26].

We propose to use Voronoi tessellations, Brillouin zones, and persistent homology to study deviations from global order. For a lattice, the persistence diagram of the Delaunay radius function is necessarily very simple, with just a few different points, each with infinite multiplicity. This suggests we characterize deviations from the global order by the effect they have on the diagram, adding new points or spreading out the piles of infinitely many copies. Similarly, the Brillouin zones for a lattice have predictable properties so that violations of these properties can be used to classify and quantify deviations from global order. For example, in a lattice the Brillouin zones approach the shape of a sphere when the depth of the zone goes to infinity. For non-lattice data, the Brillouin zones are still star-shaped so we can use the persistence diagram of the radial distance function to quantify how far its shape deviates from that of a sphere.

References

[1] F. AURENHAMMER. Power diagrams: properties, algorithms, and applications. *SIAM J. Comput.* **16** (1987) 93–105.

[2] F. AURENHAMMER. A new duality result concerning Voronoi diagrams. *Discrete Comput. Geom.* **5** (1990), 243–254.

[3] U. BAUER, M. KERBER, J. REININGHAUS AND H. WAGNER. PHAT — persistent homology algorithms toolbox. *J. Symbol. Comput.*, to appear.

[4] L. BIEBERBACH. Über die Inhaltsgleichheit der Brillouinschen Zonen. *Monatsh. Math. Phys.* **48** (1939), 509–515.

[5] L. BRILLOUIN. Les électrons dans les métaux et le classement des ondes de de Broglie correspondantes. *Comptes Rendus Hebdomadaires des Séances de l'Académie des Sciences* **191** (1930), 292.

[6] G. CARLSSON. Topology and data. *Bull. Amer. Math. Soc.* **46** (2009), 255–308.

[7] G. CARLSSON AND V. DE SILVA. Zigzag persistence. *Found. Comput. Math.* **10** (2010), 367–405.

[8] E. CHOVANCOVA, A. PAVELKA, P. BENES, O. STRNAD, J. BREZOVSKY, B. KOZLIKOVA, A. GORA, V. SUSTR, M. KLVANA, P. MEDEK, L. BIEDERMANNOVA, J. SOCHOR AND J. DAMBORSKY. CAVER 3.0: a tool for the analysis of transport pathways in dynamic protein structures. *PLOS Computational Biology* (2012), doi.org/10.1371/journal.pcbi.1002708.

[9] D. COHEN-STEINER, H. EDELSBRUNNER AND J. HARER. Stability of persistence diagrams. *Discrete Comput. Geom.* **37** (2007), 103–120.

[10] D. COHEN-STEINER, H. EDELSBRUNNER, AND D. MOROZOV. Vines and vineyards by updating persistence in linear time. In *Proc. 22nd Sympos. Comput. Geom., 2006*, 119–126.

[11] T.K. DEY. *Curve and Surface Reconstruction.* Cambridge Univ. Press, Cambridge, England, 2006.

[12] T. DEY, F. FAN AND Y. WANG. Computing topological persistence for simplicial maps. In *Proc. 30th Sympos. Comput. Geom., 2014*, 345.

[13] H. EDELSBRUNNER. The union of balls and its dual shape. *Discrete Comput. Geom.* **13** (1995), 415–440.

[14] H. EDELSBRUNNER. Surface reconstruction by wrapping finite sets in space. In *Discrete and Computational Geometry. The Goodman-Pollack Festschrift*, 379–404, eds.: B. Aronov, S. Basu, J. Pach and M. Sharir, Springer-Verlag, 2003.

[15] H. EDELSBRUNNER. Alpha shapes — a survey. In *Tessellations in the Sciences: Virtues, Techniques and Applications of Geometric Tilings*, eds.: R. van de Weygaert, G. Vegter, J. Ritzerveld and V. Icke, Springer-Verlag, to appear.

[16] H. EDELSBRUNNER AND J. L. HARER. *Computational Topology. An Introduction.* Amer. Math. Soc., Providence, Rhode Island, 2010.

[17] H. EDELSBRUNNER AND M. IGLESIAS-HAM. Multiple covers with balls I: inclusion-exclusion. *Comput. Geom. Theory Appl.* (2016), to appear.

[18] H. EDELSBRUNNER, D.G. KIRKPATRICK AND R. SEIDEL. On the shape of a set of points in the plane. *IEEE Trans. Inform. Theory* **IT-29** (1983), 551–559.

[19] H. EDELSBRUNNER, D. LETSCHER AND A. ZOMORODIAN. Topological persistence and simplification. *Discrete Comput. Geom.* **28** (2002), 511–533.

[20] H. EDELSBRUNNER AND E.P. MÜCKE. Three-dimensional alpha shapes. *ACM Trans. Graphics* **13** (1994), 43–72.

[21] H. EDELSBRUNNER AND A. NIKITENKO. Weighted Poisson–Delaunay mosaics. Manuscript, IST Austria, Klosterneuburg, Austria, 2017.

[22] H. EDELSBRUNNER, A. NIKITENKO AND M. REITZNER. Expected sizes of Poisson–Delaunay mosaics and their discrete Morse functions. *Adv. Appl. Probab.* **49** (2017), to appear.

[23] R. FORMAN. Morse theory for cell complexes. *Adv. Math.* **134** (1998), 90–145.

[24] R. FREIJ. Equivariant discrete Morse theory. *Discrete Math.* **309** (2009), 3821–3829.

[25] R. GHRIST. Barcodes: the persistent topology of data. *Bull. Amer. Math. Soc.* **45** (2007), 61–75.

[26] Y. HIRAOKA, T. NAKAMURA, A. HIRATA, E.G. ESCOLAR, K. MATSUE AND Y. NISHIURA. Hierarchical structures of amorphous solids characterized by persistent homology. *Proc. Nat. Acad. Sci. USA* **113** (2016), 7035–7040.

[27] Y.L. LEE, S.D. BARTHEL, P. DLOTKO, S.M. MOOSAVI, K. HESS AND B. SMIT. Quantifying similarity of pore-geometry in nanoporous materials. *Nature Communications* **8** (2017), doi:10.1038/ncomms15396.

[28] R.D. MACPHERSON AND D. SROLOVITZ. The von Neumann relation generalized to coarsening of three-dimensional microstructures. *Nature* **446** (2007), 1053–1055.

[29] D. MOROZOV. Welcome to Dionysus' documentation! `www.mrzv.org/software/dionysus.`

[30] M.I. SHAMOS AND D. HOEY. Closest-point problems. *In* "Proc. 16th Ann. ACM Sympos. Found. Comput. Sci., 1975", 151–162.

[31] M.M. SUHANOVSKY AND C.M. TESCHKE. Nature's favorite building block: Deciphering folding and capsid assembly of proteins with the HK97-fold. *Virology* **479-480** (2015), 487–497.

[32] A. TAUSZ, M. VEJDEMO-JOHANSSON AND H. ADAMS. JavaPlex: a research software package for persistent (co)homology. *In* "Proc. Internat. Conf. Math. Software", LNCS **8592**, eds: H. Hong and C. Yap (2014), 129–136.

[33] C. YAP AND T. DUBÉ. The exact computation paradigm. In second edition of *Computing in Euclidean Geometry*, 452–486, eds.: D.-Z. Du and F. K. Hwang, World Scientific Press, 1995.

Section b: Curriculum Vitae

Edelsbrunner, Herbert. Austrian.
Date of birth: 14. March 1958.
http://ist.ac.at/∼edels

EDUCATION AND POSITIONS

1982: Ph. D. in Technical Mathematics, Graz University of Technology, Graz, Austria.
1980: M. S. in Technical Mathematics, Graz University of Technology, Graz, Austria.

2009-present: Professor at IST Austria, Klosterneuburg, Austria.
1999-2012: Arts and Sciences Professor of Computer Science and Professor of Mathematics, Duke University, Durham, North Carolina, USA.
1985-1999: Assistant, Associate, and Full Professor of Computer Science, University of Illinois at Urbana-Champaign, Illinois, USA.
1982-1985: Assistant Professor of Information Processing, Graz University of Technology, Graz, Austria.

FELLOWSHIPS AND AWARDS

2014: Fellow of the European Association for Theoretical Computer Science.
2012, 2014: Corresponding, full member of the Austrian Academy of Science.
2009: Member of the Academia Europaea.
2008: Member of the German Academy of Science (Leopoldina).
2006: Honorary doctoral degree from the Graz University of Technology, Graz, Austria.
2005: Member of the American Academy of Arts and Sciences.
1991: Alan T. Waterman Award from the National Science Foundation, USA.

SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

I currently supervise 5 graduate students at IST Austria, two of which are expected to graduate in 2017, and have graduated 1 PhD student at IST Austria, 9 PhD students at Duke University, and 16 PhD students at the University of Illinois at Urbana-Champaign: Georg Osang (current), Katharina Ölsböck (current), Zuzana Masárová (current), Anton Nikitenko (current), Mabel Iglesias-Ham (current), Florian Pausinger (2015), Salman Parsa (2014), Brittany Fasy (2012), Ying Zheng (2012), Bei Wang (2010), Amit Patel (2010), Dmitriy Morozov (2008), Andrew Ban (2005), Vijay Natarajan (2004), Yusu Wang (2004), Ho-Lun Cheng (2001), Afra Zomorodian (2001), Damrong Guoy (2001), Ulrike Axen (1998), Michael Facello (1996), Roman Waupotitsch (1996), Patrick Moran (1996), Nataraj Akkiraju (1996), Edgar Ramos (1995), Nimish Shah (1994), Ernst Mücke (1993), Tiow Seng Tan (1992), Peter Williams (1992), Harald Rosenberger (1990), Xiaojun Shen (1989), Steve Skiena (1988).

I currently supervise 5 postdocs at IST Austria, two of which are expected to continue beyond 2017, and have in the past supervised 10 postdocs at IST Austria, 5 postdocs at Duke University, and 3 postdocs at the University of Illinois at Urbana-Champaign: Grzegorz Jabłoński (2016-present), Mirko Klukas (2015-present), Žiga Virk (2015-present), Arseniy Akopyan (2015-present), Hubert Wagner (2014-present), Pawel Pilarczyk (2014-2016), Salman Parsa (2014), Stefan Huber (2013-2015), Olga Symonova (2011-2015), Jan Reininghaus (2012-2014), Ulrich Bauer (2012-2014), Amit Patel (2010), Paul Bendich (2009-2010), Michael Kerber (2009-2012), Chao Chen (2009-2012), Yuriy Mileyko (2005-2008), David Cohen-Steiner (2003-2004), Vicky Choi (2002-2004), Alper Üngör (2002-2004), Sergej Bespamyatnikh (2001-2002), Jie Liang (1993-1996), Ernst Mücke (1993-1994), Tamal Dey (1991-1992).

TEACHING ACTIVITIES

I have taught throughout my career, including undergraduate courses in 'Data Structures' and 'Discrete Mathematics', and graduate courses in 'Algorithms', 'Probability', 'Computational Geometry', and recently 'Shapes and Patterns'. Most rewarding were research related advanced courses on topics like 'Triangulations', 'Biogeometry', and 'Computational Topology'.

COMMISSIONS OF TRUST

2016-present: Founding editor of *Journal of Applied and Computational Topology*, Springer.
2010-present: Member of Scientific Council of the Computer Science Department at the the École Normale Supérieure, Paris, France.
2010-present: Editor-in-chief of *Geometry and Computing*, a book series published by Springer.
2004-present: Editor of *Foundations of Computational Mathematics (FoCM)*, Springer.
1985-present: Editor of *Discrete and Computational Geometry (DCG)*, Springer, Editor-in-chief (2011-2015).

Appendix: All ongoing and submitted grants and funding of the PI

On-going Grants

Project title	Funding source	Amount (E)	Period	Role of the PI	Relation to current ERC project
DGD	FWF	200,000	2016–20	team leader	bridging
InfTop (pending)	ONR	220,000	2017–20	team leader	complementary
Materials (pending)	Royal Society	15,000	2017–18	one of 2 PIs	application

The full title of the FWF project is "Persistence and stability of geometric complexes", which is a sub-project of the DFG-funded Sonderforschungsbereich in "Discretization in Geometry and Dynamics". The money pays for a student at IST Austria. The project aims at building a bridge between the discrete work in our group to the discrete differential interests in the majority of the other groups in the Sonderforschungsbereich.

The full title of the ONR project is "Toward computational information topology". The money pays for one postdoc at IST Austria. The topic is complementary to this project and aims at developing computational topology tools for information theoretically motivated Bregman divergences.

The full title of the Royal Society project is "Topological data analysis for a faster discovery of new materials". The support funds visits of my group to Liverpool and visits of the Liverpool group to IST Austria. The topic is the application of computational geometry and topology to questions in material science.

Section c: Ten Years Track-Record

PUBLICATIONS

Since the year 2007, I published 38 articles in scientific journals, 9 contributions in edited book volumes, and 18 additional papers in conference proceedings. Here, I list a selection of ten journal articles.

U. BAUER AND H. E. The Morse theory of Čech and Delaunay complexes. *Trans. Amer. Math. Soc.* **369** (2017), 3741–3762. [This paper uses the formalism of generalized discrete Morse theory to give a unified view of Čech complexes, Delaunay-Čech complexes, alpha complexes, and wrap complexes. The main result is the explicit construction of a collapsing hierarchy connecting these complexes.]

H. E. G. JABLONSKI AND M. MROZEK. The persistent homology of a self-map. *Found. Comput. Math.* **15** (2015), 1213–1244. [This is the first paper to make inroads into combining the concept of persistent homology with discrete approaches to solving dynamical systems. It introduces the concept of a sampled dynamical system, which is discrete in time *and* in space, and describes algorithms that compute the persistence of the connecting maps.]

H. E., B. FASY AND G. ROTE. Add isotropic Gaussian kernels at own risk: more and more resilient modes in higher dimensions. *Discrete Comput. Geom.* **49** (2013), 797–822. [This paper analyzes under what circumstances adding Gaussian kernels gives rise to phantom modes. A key technical result is the complete analysis of the sum of such kernels placed at the vertices of a regular simplex.]

H. E. AND M. KERBER. Dual complexes of cubical subdivisions of $\mathbb{R}^n$. *Discrete Comput. Geom.* **47** (2012), 393-414. [Motivated by the importance of images in data acquisition, this paper describes combinatorial perturbations that unfold the complications caused by the non-primitive structure of cubical subdivisions. The main result is a complete analysis of the family of diagonal distortions of the integer grid in any fixed dimension.]

H. E., D. MOROZOV AND A. PATEL. Quantifying transversality by measuring robustness of intersections. *Found. Comput. Math.* **11** (2011), 345–361. [This paper uses ideas from persistent homology to quantify classically binary concept of *transversality*. A key step in the construction is one of the earliest non-trivial application of zigzag modules. The results imply a short proof of Brouwer's classic Fixed-point Theorem for balls in n dimensions.]

P. BENDICH, H. E. AND M. KERBER. Computing robustness and persistence for images. *IEEE Trans. Visual. Comput. Graphics* **16** (2010), 1251–1260. [This paper combines quad/oct-tree representations of images with the persistent homology algorithm, improving the running time by orders of magnitudes at the expense of a controlled distortion of the persistence diagram.]

D. COHEN-STEINER, H. E. AND J. HARER. Extending persistence using Poincaré and Lefschetz duality. *Found. Comput. Math.* **9** (2009), 79–103. [This paper extends the persistence diagrams to double filtrations, thus enabling applications that need finite measures of persistence for all features of a function and its domain. A key result is the description of a rich collection of symmetries the extended diagram of a function on a manifold enjoys.]

J. HEADD, Y.-H. BAN, P. BROWN, H. E., M. VAIDYA AND J. RUDOLPH. Protein-protein interfaces: properties, preferences, and projections. *J. Proteome Research* **6** (2007), 2576–2586. [This paper pushes the concept of interface surfaces in protein-protein complexes, introduces visualizations of local interactions through 2-dimensional, two-sided, and colored diagrams, and presents extensive experimental results.]

D. ATTALI AND H. E. Inclusion-exclusion formulas from independent complexes. *Discrete Comput. Geom.* **37** (2007), 59–77. [This paper introduces the concept of an *independent complex*, which relaxes Delaunay complexes by tolerating local changes of the complex structure. The main result is a proof that the inclusion-exclusion formulas for the volume of a union of balls that correspond to independent complexes are correct.]

D. COHEN-STEINER, H. E. AND J. HARER. Stability of persistence diagrams. *Discrete Comput. Geom.* **37** (2007), 103–120. [This is the first paper to formulate and prove the stability of persistence diagrams, which is considered a milestone in the development of the field. A key concept is the introduction of the bottleneck distance, which gives the space of persistence diagrams a metric space structure.]

PLENARY TALKS

Since 2007, I gave 35 plenary talks at Mathematics, Computer Science, Material Science, Geographic Information Systems, and Astronomy meetings. Here, I list a selection of ten meetings.

2017: SIAM Conf. Applied Algebraic Geometry, Atlanta, Georgia.
2016: Tetrahedron V: 5th Workshop on Grid Generation for Numerical Computations, Liège, Belgium.
2016: 11th Internat. Comput. Sci. Sympos. in Russia, St. Petersburg, Russia.
2015: 23rd Internat. Sympos. Graph Drawing and Network Visualization, Los Angeles, California.
2015: IAMR Internat. Sympos., Sendai, Japan.
2014: 8th Internat. Conf. Geographic Information Science, Vienna, Austria.
2014: 25th ACM-SIAM Sympos. Discrete Algorithms, Portland, Oregon.
2012: 6th Europ. Congress Math., Krakow, Poland.
2010: 6th Conference on Astronomical Data Analysis, Montasir, Tunesia.
2007: 6th International Congress on Industrial and Applied Mathematics. Zürich, Switzerland.

DISTINGUISHED LECTURES

Since 2007, I delivered 9 distinguished lectures at Universities in the US, Europe, and Asia. Here, I list a selection of five.

2014: Distinguished Lecturer Series, Ohio State University, Columbus, Ohio.
2012: College of France, Paris, France.
2011: Academia Sinica, Institute of Information Science, Taipei, Taiwan.
2010: Applied Mathematics and Computational Science, University of Pennsylvania, Philadelphia.
2008: Distinguished Lectures in Computer Science, Columbia University, New York.

CITATIONS

Google Scholar found 31,918 citations in total, with h-index 81, and i10-index 224. Since 2012, it found 10,038 citations, with h-index 44, and i10-index 133.