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Topological Methods in Data Analysis and Visualization

Theory, Algorithms, and Applications

With 146 Figures, 122 in Color

Springer
Preface

The deluge of data observed throughout research and industry has turned the analysis of the resulting information into the primary limiting factor for the rapid progress of science, engineering, and medicine. The field of visualization strives to tackle this data analysis challenge by devising visual representations that afford users an effective interface with their datasets. Driven by the explosion in data size and complexity experienced over the last decade, a prominent trend in today’s visualization research applies a data abstraction approach to yield high-level depictions emphasizing various salient properties of the phenomenon considered. Topology-based methods have proved especially compelling in this regard, as the topological abstraction provides a common mathematical language to identify remarkable structures in a broad range of applications and semantic contexts. Topological concepts and metaphors are therefore permeating the visualization literature and they are the focus of a significant research effort spanning theoretical, algorithmic, and practical aspects.

This book describes the research that was presented during the third Workshop on Topological Methods in Data Analysis and Visualization, which took place in Snowbird, Utah, on February 23-24, 2009. Following two successful, seminal TopoInVis workshops held in Europe, the 2009 edition was organized in the United States in response to the growing international interest in topological methods. As in previous years, this event offered international experts the opportunity to present their ongoing research in an informal and inspiring atmosphere, as well as to discuss the emerging trends and open challenges of the field. A defining feature of the 2009 edition was the attention paid to applications, reflecting the importance of topological techniques in practical data analysis scenarios and the increased prominence of problem-driven research. The workshop featured two eminent invited speakers (Herbert Edelsbrunner, Duke University, and Jackie Chen, Sandia National Laboratory), who gave exciting lectures highlighting significant accomplishments and promising avenues for both fundamental and applied research on topological methods. All in all, TopoInVis ’09 was a resounding success thanks to the excellent contributions of over 60 participants.

Each of the 20 research papers contained in this book was accepted for presentation at the workshop after careful peer-review by the international program committee. The contents are organized in 5 main themes that correspond to major research directions.

The first part is concerned with the theoretical foundations of the topological approach. Jordan et al. apply topological concepts to the precise visualization of 1-manifolds, while Kälberer et al. employ the topology of a tubular surface to define a globally consistent stripe texture. Edelsbrunner and his co-authors prove the stability of apparent contours (i.e. silhouettes) under the erosion distance and Dillard et al. study the topologically consistent reconstruction of cell complexes from cross-section images.

The second part of the book focuses on hierarchical topological data structures, as required by the analysis of very large datasets. Vivodtzev et al. present a new technique for the topology-preserving simplification of very large tetrahedral meshes. Guylassy et al. propose several improvements to the computation of Morse-Smale complexes in the context of feature detection algorithms, while Comić and De Floriani introduce
two simplification operators for Morse complexes applicable in arbitrary dimensions. Suthambhara and Natarajan consider the simplification of Jacobi sets from a level set and offset manifold perspective, and Reininghaus and Hotz describe a novel combinatorial framework for the topological analysis of 2D vector fields.

The third part deals with the algorithmic extraction of topological structures of interest in vector and tensor fields. Kasten et al. put forward a Galilean invariant notion of critical points that captures significant patterns in turbulent flows, while Obermaier and his co-authors propose an algorithm for the segmentation of three-dimensional grid-less flow simulations. Sreevalsan-Nair et al. study the impact of the interpolation scheme on the topological structure of 2D eigenvector fields. Finally, Sadlo et al. present a new method for the efficient computation of Lagrangian coherent structures in unsteady flows.

The following part is dedicated to practical applications of topological methods in data analysis and visualization. Grottel et al. consider defect detection in crystal structures; Keller and his co-authors apply a user-assisted multi-scale technique to the detection of salient features in LiDaR datasets. Wiebel et al. report on the shortcomings of existing topological approaches in the analysis of rotation-mediated cell aggregation and propose a novel solution to this problem. Szymczak applies category theory to the robust segmentation of airways from CT scans, while Bajaj and his co-authors visualize the complementary space of complex geometric models to resolve subtle structures with applications to uncertainty and dynamics visualization.

The book concludes with two papers that specifically consider the challenges posed by the topological analysis of very large datasets produced by state of the art combustion simulations. Mascarenhas et al. present a combinatorial streaming algorithm for the efficient characterization of topological features in large-scale datasets, which they apply to the comparison of terascale combustion simulations. Weber and his co-authors propose a novel technique, leveraging Reeb graphs to study the temporal evolution of burning regions in simulated flames.

Acknowledgments

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Valerio Pascucci
Xavier Tricoche
Hans Hagen
Julien Tierny
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Abstract: Ambient isotopic approximations are fundamental for correct representation of the embedding of geometric objects in $\mathbb{R}^3$, with a detailed geometric construction given here. Using that geometry, an algorithm is presented for efficient update of these isotopic approximations for dynamic visualization with a molecular simulation.

1 Approximation and Topology for Visualization

Figure 1(a) depicts a knot\(^5\) and Figure 1(b) shows a visually similar protein model\(^6\), prompting two criteria for efficient algorithms for visualization:

- a piecewise linear (PL) approximation that preserves model topology.
- preservation of topology during dynamic changes, such as protein unfolding.

The visual comparison from Figure 1 led to invoking knot theory to provide the unifying mathematics. This paper presents a curvature-adaptive, topology preserving approximation for a parametric 1-manifold with the primary result being Theorem 3. The piecewise linear (PL) approximations presented will

(i) be topologically equivalent to the original manifold,
(ii) minimize the number of linear approximants,
(iii) respect user-specified error bounds for distance & curvature.

While many approximation methods fulfill criteria (ii) and (iii), the stipulation of criterion (i) is of recent interest and the methods here are for a rich class of curves, extending related results. The topological equivalence chosen for dynamic molecular visualizations is by ambient isotopy, as this preserves the embedding of the geometric model over time.

**Definition 1.** Let $X$ and $Y$ be two subsets of $n$-dimensional space $\mathbb{R}^n$. An ambient isotopy is a continuous function $H : \mathbb{R}^n \times [0, 1] \rightarrow \mathbb{R}^n$ such that

1. $H(\cdot, 0)$ is the identity function,
2. $H(X, 1) = Y$, and
3. For each $t$ in $[0, 1]$, $H(\cdot, t)$ is a homeomorphism on $\mathbb{R}^n$.

**2 Related Work**

Preliminary work by some of these authors and collaborators has appeared: for the integration of time and topology in animations and simulations [12] and for isotopic approximations on various classes of spline curves [14–17]. The theory presented here extends to a broad class of parametric curves that properly includes splines. While one approximation method could be applied to general parametric curves [12] the isotopy results within that paper relied upon Bézier geometry.

The proof techniques for isotopy here are a slight variant of the well-known ‘push’ from geometric topology for a 3-manifold [2]. The importance for applications is the creation of explicit neighborhoods within which the approximant can be perturbed while remaining ambient isotopic. These can serve as the basis for determining efficient updates for these isotopic constraints during dynamic visualizations.

A previous application of these tubular neighborhoods has emphasized visualizing knots undergoing dynamic changes [4]. Another tubular neighborhood algorithm [14] for rational spline curves [19] relies upon specialized numerical solution software, whereas computation with Newton’s method has been exhibited on Bézier curves [15, 16]. Related treatments to curve approximations are available: within Hilbert spaces [10], with restrictions to planar curves [8] or specialized to spline curves [18]. The approach of approximating with respect to curvature is similar to an approach for ‘aesthetic engineering’ [20].

This terse summary on curve approximation stresses only the most relevant literature, as any comprehensive survey would be voluminous, with one indication being that a literature search on curve approximation resulted in 1.4 million hits\(^7\). The distinguishing feature, here, is the additional insistence of topological equivalence. This emphasis upon geometric topology is appropriate when a geometric model is present, as for the molecular models discussed, and could prove complementary to other uses of topology in visualization that depend largely upon algebraic topology [6, 7].

\(^7\)http://scholar.google.com/
3 Curvature & Topology for Parametric 1-Manifolds

Each curve considered here is assumed to be a compact 1-manifold, thereby excluding
self-intersections, where stated differentiability assumptions also preclude wild arcs\(^8\). Further, each 1-manifold is assumed to be parameterized by arc length over the unit\(^9\) interval.

**Notation:** Let \(c : [0, 1] \to \mathbb{R}^3\) be a \(C^3\) curve and we denote

\[
\mu_c([a, b]) = \int_a^b ||c''(t)||dt,
\]

which will be invoked as the basis for our curvature-adaptive approximation.

**Theorem 1.** Let \(c : [0, 1] \to \mathbb{R}^3\) be a \(C^3\) curve. For each \(\varepsilon > 0\), there exists a natural number \(n\) and a partition \(X = \{p_1, \ldots, p_n\} \subseteq [0, 1]\) such that, for \(i = 1, \ldots, n\), \(p_1 = 0, p_n = 1; p_1 < p_2 < \ldots < p_{n-1} < p_n;\) and

\[
\int_{p_i}^{p_{i+1}} ||c''(z)||dz = \mu_c([p_i, p_{i+1}]) < \varepsilon,
\]

there is a set of compact cylinders \(\{C_i\}_{i=1}^n\), such that each \(C_i\) has its axis aligned with the tangent at \(c(p_i)\) and has radius \(\varepsilon\). Furthermore both the polyline formed by consecutively connecting the vertices \(\{c(p_i) : i = 1, \ldots, n\}\) and the curve \(c\) lie in \(\bigcup_{i=1}^n C_i\).

Theorem 1 can be used to create a PL approximation of a curve, but there are no guarantees given that the approximant is topologically equivalent to the original curve. Further constraints must be imposed upon the choice of \(\varepsilon\) to ensure that the approximant produced is ambient isotopic to the original curve, as will be developed in the rest of this paper. The proof of Theorem 1 follows.

**Proof.** We construct one cylinder \(C_i\) for each point in the set \(X\). Let \(L_i\) be the line containing the vector \(c'(p_i)\). Consider the plane normal to \(c'(p_{i+1})\). This plane intersects \(L_i\) at a point, denoted as \(q\). Define \(C_i\) to be the cylinder of radius \(\varepsilon\) whose axis is the portion of \(L_i\) connecting \(p_i\) and \(q\). By Taylor's Theorem if \(t \in [p_i, p_{i+1}]\) then

\[
|c(t) - c(p_i) - (t - p_i)c'(p_i)| \leq \int_{p_i}^{t} ||c''(z)||dz \leq \int_{p_i}^{p_{i+1}} ||c''(z)||dz < \varepsilon.
\]

Hence, \(c(t)\) is of distance at most \(\varepsilon\) from \(c(p_i) + (t - p_i)c'(p_i)\). Thus \(c(t)\) is at most \(\varepsilon\) away from \(L_i\), and so \(c(t)\) is in the cylinder \(C_i\). The last statement is clear as each cylinder is convex and the endpoints \(c(p_i), c(p_{i+1})\) of an approximating segment are contained in the cylinder \(C_i\).

\(^8\)Any \(C^2\) compact 1-manifold is tame [14].

\(^9\)If not of unit length, scale accordingly.
If, for each $i$, Inequality 1 is modified so that $\mu_c([p_i, p_{i+1}]) = \varepsilon$, then a previously published proof [12] can be applied for an asymptotic limit on the number of segments in the approximation. For $\varepsilon > 0$, denote by $N(\varepsilon)$ the number of cylinders given by the construction in the proof of Theorem 1.

**Corollary 1.** If $c$ is also $C^3$ such that $||c''(t)|| > 0$ for all $t$, then

$$\lim_{\varepsilon \to 0} \sqrt{\varepsilon} \cdot N(\varepsilon) = \int_0^1 \sqrt{||c''(u)||} du.$$

We identify important properties studied in geometric topology and prove maintenance of those characteristics for the approximant. For the remainder of the section we will refer to the set $X = \{p_1, \ldots, p_n\}$ where the $p_i$'s are ordered as described, above, and the cylinders $C_i$ are constructed as in Theorem 1. We ensure that the curve is well-behaved within each cylinder through the following lemmas.

**Lemma 1.** Let $c : [0, 1] \to \mathbb{R}^3$ be a $C^3$ curve and $r, s \in [p_i, p_{i+1}]$, then

$$||c'(r) - c'(s)|| \leq \sqrt{3} \varepsilon.$$

**Proof.** For $t \in [0, 1]$ denote by $c'(t)_x$ the x-coordinate for $c'(t)$. We can apply Taylor’s Theorem to see for $r, s \in [p_i, p_{i+1}]$,

$$|c'(r)_x - c'(s)_x| \leq \int_r^s |c''(u)_x| du \leq \int_r^s ||c''(u)|| du \leq \varepsilon.$$

The case is similar for the $y$ and $z$ coordinates, and the result follows.

**Corollary 2.** Let $c : [0, 1] \to \mathbb{R}^3$ be a $C^3$ space curve, and $\varepsilon < \sqrt{2/3}$. Then for points $r, s \in [p_i, p_{i+1}]$ the tangential deviation between $c'(r)$ and $c'(s)$ is no more than $\pi/2$.

**Proof.** Since we are parameterized using arc length, we have $||c'(r)|| = ||c'(s)|| = 1$ for any $r, s \in [p_i, p_{i+1}]$. Further, by Lemma 1,

$$||c'(r) - c'(s)|| < \sqrt{3} \varepsilon.$$

The Law of Cosines shows the angle between them is $\arccos(1 - \frac{3}{2} \varepsilon^2)$. When $\varepsilon < \sqrt{\frac{2}{3}}$, we have $\arccos(1 - \frac{3}{2} \varepsilon^2) < \frac{\pi}{2}$.

So we can explicitly control the tangential deviation within each cylinder $C_i$. The benefit here is that we can use this information to control intersections within each cylinder.

**Lemma 2.** Let $c : [0, 1] \to \mathbb{R}^3$ be a $C^3$ curve and $[a, b] \subset [0, 1]$. Assume all of the tangent vectors of the subcurve $c([a, b])$ deviate in angle by no more than $\eta < \frac{\pi}{2}$ from a particular tangent vector $c'(t)$ for $t \in [a, b]$. If $\Pi$ is a plane with normal $c'(t)$ and $\Pi \cap c([a, b]) \neq \emptyset$, then $|c([a, b]) \cap \Pi| = 1$. 

Proof. Orient the plane II so that it is parallel with the xy-plane and \( c'(t) \) with the positive z-axis. In this orientation if \( c'(r)_z = 0 \) for any \( r \in [a,b] \) then \( c'(r) \) is parallel to the plane II and this would be a contradiction as \( c'(t) \) is normal to the plane II and the angular deviation of tangent vectors is not more than \( \frac{\pi}{4} \). For any \( s \in [a,b] \) with \( s \neq t \), if \( c(s) \) lies on the plane II then \( c(s)_z = 0 \) and since \( c(t)_z = 0 \) we have, by the Mean Value Theorem, another point \( r \) with \( c'(r)_z = 0 \), which is a contradiction.

**Notation:** For the remainder of this paper, let

- \( c : [0,1] \rightarrow \mathbf{R}^3 \) denote a \( C^3 \) curve,
- \( \kappa = \max \|c''(z)\|, \alpha = \min \{1, ||c''(z)||\} \),
- \( X \) be a set which satisfies the hypothesis of Theorem 1, and
- For \( p_i, p_{i+1} \in X \), let \( c_i = c([p_i, p_{i+1}]) \).

Our next step is to construct sets upon which we can build local isotopies between the curve and the approximant. In order to do this we will make use of Taylor’s theorem, as in the following lemma.

**Lemma 3.** Let \( \gamma \) be chosen such that \( \gamma > 0 \), but \( \gamma \ll (\kappa/2)(t-p_i)^2 \). For \( t \in (p_i, p_{i+1}] \), let \( S_t \) be the closed ball with center \( c(p_i) + (t-p_i)c'(p_i) \) and radius \( r_t \), with \( r_t = (\kappa/2)(t-p_i)^2 + \gamma \). Then, \( c(t) \in \text{int}(S_t) \).

**Proof.** By Taylor’s theorem we have

\[
\|c(t) - c(p_i) - (t-p_i)c'(p_i)\| \leq \int_{p_i}^{t} ||c''(z)|| (t-z) dz \\
\leq \kappa [t^2 - (1/2)t^2 - (tp_i - (1/2)p_i^2)].
\]

However \( t^2 - (1/2)t^2 - (tp_i - (1/2)p_i^2) = (1/2)(t-p_i)^2 \). The use of \( \gamma \) permits the conclusion about containment in the interior.

For each \( t \in (p_i, p_{i+1}] \), define a ‘snowcone’ \( K_t \) as the convex hull* of \( S_t \) and \( \{p_i\} \), where the use of the colloquial term ‘snowcone’ is meant to suggest the compact set created, with a planar cross-section shown in Figure 2. The next lemma shows the relationship between the opening angle of these snowcones** for different values \( t \).

**Lemma 4.** Choose \( \varepsilon \in (0, \alpha/(2\kappa)) \). Let \( t \in (p_i, p_{i+1}] \), let \( \theta_t \) be opening angle at \( c(p_i) \) for \( K_t \). Then \( \theta_t \) is an increasing function of \( t \) and each snowcone \( K_t \), for \( t \in (p_i, p_{i+1}] \), is contained in the snowcone \( K_{p_{i+1}} \).

---

*For any two sets \( A \) and \( B \), their convex hull is defined as the smallest convex set that contains \( A \cup B \).

**In the United States, a frozen desert having a two dimensional profile similar to that of Figure 2 is known as a ‘snowcone’.

---
Proof. Denote by \( r_t = \left( \frac{\kappa}{2} \right) (t - p_i)^2 \) the radius of \( S_t \). Since
\[
\int_{p_i}^{p_{i+1}} ||c''(z)|| dz < \varepsilon
\]
we have that \( \alpha(p_{i+1} - p_i) < \varepsilon \) and since \( \varepsilon < (2\alpha/\kappa) \) we have that
\[
(t - p_i) \leq (p_{i+1} - p_i) \leq \varepsilon/\alpha \leq 2/\kappa.
\]
Thus, \( (\kappa/2)(t - p_i) \leq 1 \) and \( (\kappa/2)(t - p_i)^2 \leq (t - p_i) \). Therefore, \( c(p_i) \) is not contained in the sphere \( S_t \). Consider a planar cross section of the snowcone \( K_t \) and within this planar cross section, choose a tangent to \( S_t \) and denote the point of tangency as \( v \). Denote the angle between \( c'(p_i) \) and the segment \([c(p_i), v]\) by \( \theta \). Denote by \( z \) the center of \( S_t \). Using the triangle defined by \( z, v, c(p_i) \) one can conclude that \( \sin \theta_t = r_t/(t - p_i) = (\kappa/2)(t - p_i) \). For reference, consider Figure 2. Since \( r_t \) is finite, \( \theta_t < \pi/2 \). For \( t, s \in [p_i, p_{i+1}] \) with \( t < s \), \( \sin \theta_t < \sin \theta_s \) and so \( \theta_t < \theta_s \), as \( \theta_s < \pi/2 \).

![Fig. 2. Cross section of snowcone \( K_t \)](image)

Hence, for \( t \in (p_i, p_{i+1}] \), \( K_t \subset K_{p_{i+1}} \).

Corollary 3. The snowcone \( K_{p_{i+1}} \) contains \( c_i \).

Proof. First note that \( c(p_i) \in K_{p_{i+1}} \) as it is the apex of this snowcone. For each \( t \in (p_i, p_{i+1}], c(t) \in K_{p_{i+1}} \) by Lemmas 3 and 4.

Notation: First, modify the existing notation \( K_{p_{i+1}} \) to be \( K_{t_{i+1}} \), using the order of these subscripts to express that the snowcone’s apex is at \( p_t \) and opens towards \( p_{t+1} \). This is to contrast it with a similar snowcone, denoted as \( K_{t_{i+1}, t} \), which will have its apex as the point \( c(p_{i+1}) \), its axis as the line containing \( c'(p_{i+1}) \) but will open towards \( p_i \), as indicated in Figure 3.
Lemma 5. For each \( i = 1, \ldots, n - 1 \), denote the approximating segment connecting the points \( c(p_i) \) and \( c(p_{i+1}) \) by \( a_{i,i+1} \). For each cylinder \( C_i \), there is a convex subset of \( C_i \), denoted \( V_{i,i+1} \), containing \( c_i \), such that
\[
V_{i,i+1} \cap V_{i+1,i+2} = c(p_{i+1}).
\]

Proof. Define \( V_{i,i+1} = K_{i,i+1} \cap C_i \cap K_{i+1,i} \). Since each of the intersecting sets is convex, it is clear that \( V_{i,i+1} \) is convex. But then, since both \( c(p_i) \) and \( c(p_{i+1}) \) are in \( V_{i,i+1} \), it is clear that \( a_i \subset V_{i,i+1} \). From Corollary 3, \( c_i \subset V_{i,i+1} \).

4 Building the Ambient Isotopy

The results so far only provide local views on \( c \) by focusing on each \( c_i \) independently. It is often easy to build an isotopy locally on one portion of a curve, but considerable subtlety can be required to unify these into an isotopy of the entire curve. The snowcones were defined for use in an iterative algorithm to establish an ambient isotopy for all of \( c \).

Outline of Algorithm for Entire Curve: The geometric objective for the algorithm is to continue to reduce the radius of each cylinder \( C_i \) used in defining the sets \( V_{i,i+1} \) until the interiors of these \( V_{i,i+1} \) are pairwise disjoint, that is, for \( i \neq j \),
\[
\text{int}(V_{i,i+1}) \cap \text{int}(V_{j,j+1}) = \emptyset.
\]

The algorithm begins with a seed value for \( \delta \) to construct a set \( X_1 \) such that for each \( i = 1, \ldots, n \), and \( p_i, p_{i+1} \in X_1 \), we have \( \mu_c([p_i, p_{i+1}]) < \delta \). The algorithm proceeds by replacing the value of \( \delta \) by \( \delta/2 \), so that at each successive iteration \( j \), the set \( X_j \) has
the above mentioned containment properties relative to the current value of $\delta$. The algorithm proceeds until these bounding volumes are pairwise disjoint in order to form an isotopy of the entire curve. A previously published termination proof [15] can be easily modified for this snowcone geometry. Indeed, the more aggressive containment snowcone geometry used here actually simplifies the previous proof, so that both algorithms terminate in $O(\log \Delta^{-1})$ iterations [15], where $\Delta$ is the minimum separation distance of the curve. For the curve $c$, define $d : [0, 1] \to \mathbb{R}$ to be the distance function $d \equiv \|c(s) - c(t)\|$. Then the minimum separation distance is the minimum critical value of $d$. A useful geometric formulation of this problem is to find all pairs of distinct points at parametric values $s$ and $t$ of $c$ to satisfy the equations [13]:

\begin{equation}
(c(s) - c(t)) \cdot c'(s) = 0
\end{equation}

\begin{equation}
(c(s) - c(t)) \cdot c'(t) = 0.
\end{equation}

Recent approaches to efficiently solve these simultaneous Equations 2 and 3 have appeared [15]. The value of $\Delta$ is then the minimum Euclidean distance over all pairs $(c(s), c(t))$ that are solutions to these simultaneous equations. The role of $\Delta$ as a stopping criterion can be intuitively expressed as measuring the minimum Euclidean distance between points of $c$ that can be geodesically far apart. The algorithm restricts the size of the snowcones relative to $\Delta$.

We first build a local homeomorphism on $c_i$ and use that as a basis for constructing an ambient isotopy over all of $c$. For each point $w \in c_i$, let $N_w$ denote the normal plane to $c_i$ at $w$. Choose $\epsilon$, in accordance with Corollary 2 to ensure that tangents on $c_i$ deviate by less than $\pi/2$. Define the function

$$h_i : c_i \to a_{i,i+1}$$

by

$$h_i(w)$$ is the single point in $N_w \cap a_{i,i+1}$.

**Theorem 2.** The function $h_i$ is a homeomorphism that fixes both $c(p_i)$ and $c(p_{i+1})$.

**Proof.** We consider the intersection of each $N_w$ and $a_{i,i+1}$.

First, suppose that $a_{i,i+1}$ is a subset of $N_w$, requiring that both end points of $a_{i,i+1}$ were in $N_w$. But these end points are also points of $c_i$, which would be a contradiction to Lemma 2. If $w$ is either endpoint of $c_i$, then it is also a point of $a_{i,i+1}$, but then Lemma 2 provides that this endpoint is the only element of the $N_w \cap a_{i,i+1}$.

So, suppose $w$ is not an endpoint, then $c(p_i)$ cannot also be in $N_w$, by Lemma 2, and, similarly, $c(p_{i+1})$ cannot be in $N_w$. But, then, since $\pi/2$ is an upper bound on the tangents on $c_i$, it is clear that $c(p_i)$ and $c(p_{i+1})$ must be on opposite sides of $N_w$. So, $a_{i,i+1}$ and $N_w$ cannot be disjoint. But, then, $N_w$ and $a_{i,i+1}$ intersect in a single point, since a plane and a line can intersect only in the line itself or in a single point.

Then $h_i$ is a well-defined function on each $c_i$, where continuity is obvious. Moreover, note that $h_i$ keeps the end points of $c_i$ fixed. That $h_i$ is onto follows since the endpoints of $a_{i,i+1}$ remain fixed and the image of $h_i$ is a connected subset of $a_{i,i+1}$. That $h_i$ is 1-1 follows, since $a_{i,i+1}$ is within $\epsilon$ of $c_i$, with $\epsilon$ chosen to be less than $1/(2\kappa)$ (with $\kappa$ chosen to be the maximum curvature) so, the line segments given by $[w_1, h(w_1)]$ and $[w_2, h(w_2)]$ do not intersect.
Now we are set to define a local isotopy within the bounding volume $V_{i,i+1}$. But first we need to recall some easily proven properties of convex sets of $\mathbb{R}^n$. Let $A$ denote a non-empty, compact, convex subset of $\mathbb{R}^n$, for some positive integer $n$.

**Lemma 6.** For each point $p \in \text{int}(A)$ and $b \in \partial A$, the ray going from $p$ to $b$ only intersects $\partial A$ at $b$ (See Figure 4(a).)

Fig. 4. (a) Rays outward.  (b) Variant of a push.

**Lemma 7.** Let $A$ be a compact convex subset of $\mathbb{R}^2$ with non-empty interior and fix $p \in \text{int}(A)$. For each boundary point $b \in \partial A$, denote by $[p,b]$ the line segment from $p$ to $b$. Then $A = \bigcup_{b \in \partial A} [p,b]$.

Many of the arguments of the proof of Theorem 2 can be adapted to build the ambient isotopy of $c$. The construction relies strongly on having a compact, convex set of support, as illustrated in Figure 4(b). The previous attention to convexity of $V_{i,i+1}$ was directed towards this construction.

**Corollary 4.** There is an ambient isotopy of $c_i$, with compact support $V_{i,i+1}$ that takes each point of $c_i$ to $h(c_i)$.

**Proof.** A value of $\varepsilon > 0$ should be chosen so that $\varepsilon < \sqrt{2/3}$ to fulfill the conditions of Corollary 2 so that each $h_i$ is a homeomorphism. Simultaneously choose, $\varepsilon < \alpha/(2\kappa)$ to satisfy the hypotheses of Lemma 4 while also constraining $\varepsilon \leq \delta$ to ensure that the interiors of the bounding volumes $V_{i,i+1}$ and $V_{j,j+1}$ are disjoint, with $\delta$ being the output of the iterative algorithm outlined at the beginning of this section. It should be clear that bounding volumes $V_{i,i+1}$ and $V_{i+1,i+2}$ intersect only at the point $c(p_{i+1})$.

The proof is a variant of a ‘push’ [2], where point $p$ and $q$ are in the interior of a non-empty, convex, planar set. As illustrated in Figure 4(b), each point $v$ on a line segment between $p$ and a boundary point $b$ is mapped by linear interpolation onto the segment $[q,b]$, as $p$ is mapped onto $q$, and then Lemmas 6 and 7 are applied to build the ambient isotopy from the homeomorphism of Theorem 2.
Theorem 3. There is an ambient isotopy of $c$ onto its PL approximant $a$ and this isotopy has compact support $\bigcup_i V_{i,i+1}$.

Proof. The snowcone construction leaves bounding volumes $V_{i,i+1}$ and $V_{i+1,i+2}$ intersecting only at the point $p_{i+1}$, which is fixed under the local isotopy, so a ‘pasting lemma’ [16] can be applied to complete the proof.

5 Conclusions and Future Work

The primary result of this work is a curvature-adaptive, ambient isotopic approximation for a 1-manifold, inclusive of distance and tangency error bounds on the approximant. The bounding volumes also constrain many isotopic movements of the approximant curve.

The image of Figure 1(a) is the first frame of an animation showing that curve deforming under the application of energy described by Gaussian functionals, with guarantees that the embedded topology is preserved during this process. Similarly, the long-term focus here is to produce dynamic visualization of complex molecules undergoing simulated deformations under energy and chemical changes that also preserve the embedded topology. The essential first step is to produce a topology-preserving approximation of the static model. A specific approximated geometry model might be able to have multiple ambient isotopic perturbations within its bounding volume. However, if successive movements have the approximated geometry approaching the boundaries of the bounding volumes, new bounding volumes need to be computed. As long as the curve remains $C^2$ the existence of these new bounding volumes is known from classical differential topology [11].

However, those existence theorems typically do not provide explicit bounding geometry and they are not necessarily adaptive in the sense shown here. The value provided here is the detailed geometric constructions can be used to create algorithms that will allow for efficient updates of the geometric bounding neighborhoods as fundamental for dynamic visualization. The algorithm outlined in the second paragraph of Section 4 can be refined further, dependant upon the specific models being considered, for even more aggressive bounding volumes, when geometric alternatives to the snowcones used here might be useful on specific data.

In Figure 1(b), there was considerable empty space around the geometric model being unfolded, but Figure 5 depicts a very dense configuration. The control for isotopies can become quite delicate for molecular models. In Figure 5, the close geometric proximity and associated small bounding volumes will require updates after even small movements. This model has been the subject of consideration for dynamic visualization of molecular simulation [12] and is the current test case for algorithmic performance. The geometry in Figure 5 is also multi-dimensional, but the geometric topology used has well-known generalizations beyond dimension one. Guidance for extension to higher dimensions may be gained by considering other papers on topological approximation of 2-manifolds [1, 3, 5, 9]. A particularly relevant

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comparison is to recent results focusing on a sufficiently dense set of sample points [5] to give both error bounds and topological guarantees.

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References


Abstract. We present a novel algorithm for automatic parameterization of tube-like surfaces of arbitrary genus, such as the surfaces of knots, trees, blood vessels, neurons, or any tubular graph with a globally consistent stripe texture. Mathematically, these surfaces can be described as thickened graphs, and the calculated parameterization stripe will follow either around the tube, along the underlying graph, a spiraling combination of both, or obey an arbitrary texture map whose charts have a 180 degree symmetry.

We use the principal curvature frame field of the underlying tube-like surface to guide the creation of a global, topologically consistent stripe parameterization of the surface. Our algorithm extends the QuadCover algorithm and is based, first, on the use of so-called projective vector fields instead of frame fields, and second, on different types of branch points. That does not only simplify the mathematical theory, but also reduces computation time by the decomposition of the underlying stiffness matrices.

1 Introduction

Tubular surfaces appear in many application areas such as networks of blood vessels and neurons in medicine, or tube and hose systems in industrial environments. Often a tubular structure must be recovered and segmented from noisy scan data. Our stripe parameterizer is an efficient and automatic method for the parameterization and remeshing of free-form tubular surfaces given as triangle meshes. Our special focus lies on free-form surfaces which are not made out of regular, cylindrical tube pieces - those can be handled better by other algorithms from CAD. An additional benefit of the stripe parameterization is the enhanced visualization of the underlying geometric structure.

1.1 Previous work

Surface parameterization is an active research area. We will not attempt a complete review of the literature but instead refer the reader to the surveys by Floater and Hormann [6] and [11].

A very early surface parameterization method is the Tutte’s [24] barycentric graph embedding. Tutte embeddings are of combinatorial structure and do not capture the geometry of the surface. Early global parameterization methods were introduced by Haker, Gu and Yau [8,9,13] who studied conformal parameterizations. Conformal maps are angle preserving at the cost of possibly large length distortions, as angles and lengths can not be preserved at the same time.

To reduce length distortion, Kharevych et al. [16] used cone singularities for conformal parameterization, which relax the constraint of a flat parameter domain at few
isolated points. Such singularities have proven to be essential for high quality parameterizations and have been used in other parameterization schemes as well.

Tong et al. [23] use singularities at the vertices of a hand-picked quadrilateral meta layout on the surface. The patches the meta layout are then parameterized by solving for a global harmonic one form. Dong et al. [3] use a similar idea for parameterization but create the quadrilateral meta layout automatically from the Morse-Smale complex of eigenfunctions of the mesh Laplacian.

Ray et al. [21] parameterize surfaces of arbitrary genus with periodic potential functions guided by two orthogonal input vector fields. This leads to a continuous parameterization except in the vicinity of singular points on the surface. These singular regions are detected and reparameterized afterwards. With the QuadCover algorithm [15] we built upon their idea to use an input field as guiding directions for parameter lines. Input fields can be principal curvature directions, for example, or user-designed fields using one of the recent tools for the design of rotational symmetry fields like [22], [18], [25], or [17]. The idea of QuadCover is to find a parameterization whose gradient matches the input directions as well as possible.

The literature on parameterization of tubular objects is by far not as extensive as for general surfaces. Huysmans et al. [12] construct a progressive mesh which they map to an open cylinder. A subsequent iterative scheme optimizes the vertex positions in the cylindrical domain. Unfortunately, that method can not handle bifurcations. Antiga and Steinman [1] handle blood vessels with bifurcations by splitting the vessel tubes at their branches, and parameterize each segment separately which leaves visible artifacts at the joints of the segments. Zhu et al. [26] use conformal parameterizations on tubular objects. Since conformal maps do not allow precise control over the direction of parameter lines, they cannot be aligned with the tube axis.

1.2 Contributions

We introduce the stripe parameterizer, an algorithm for the generation of globally consistent stripe parameterizations, see Fig. 1 and 9. Each parameterization is a collection of texture maps which may also be used to remesh and segment a surface. The stripe parameterizer is a generalization of QuadCover, which parameterizes general surface meshes. The stripe parameterizer allows to map stripe patterns onto a surface, i.e., texture maps whose individual charts are symmetric with respect to rotations of 180 degrees. In contrast to QuadCover, where all texture image charts have to be symmetric with respect to 90 degree rotations, the stripe parameterizer allows a more general set of texture images with only 180 degree symmetry.

We develop the mathematical theory for stripe parameterizations and discuss the differences to grid parameterization techniques including those in QuadCover. Stripe parameterizations allows only a subset of the branch point types of QuadCover. For example, cone points of index 1/4 at the corners of a cube can not be used in stripe parameterizations since 90 degree rotational symmetric textures charts would be required, see the cube in Fig. 2.

Only one type of branch points can occur on a 2-sheeted covering, so there is no need to handle different branch types. The 4-sheeted branched covering surface from QuadCover projects onto a unique 2-sheeted branched covering surface for the stripe
parameterizer. Furthermore, the stiffness matrix from QuadCover decomposes into two matrices of quarter size. Thus, the numerical effort of computing a stripe parameterization is seriously reduced.

We tested the stripe parameterizer on several test models and real world examples including clinical data and various tree-like surfaces.

![Tree with stripe parameterization. Singularities are marked in green. The texture image consists of a vertical stripe visualizing the $u$-isolines of the parameterization.](image)

### 2 Overview

A stripe parameterization is a special case of a $(u, v)$-parameterization, where the parameter lines can be globally separated into $u$-lines and $v$-lines, as in Fig. 1. This separation property is not present on general surfaces if singularities of quarter index are present.

Stripe parameterizations can be used for mapping texture images which are symmetric by rotations of 180 but not necessarily 90 degrees, such as stripe textures. An example of a parameterization which is not suitable for mapping stripe textures is shown in Fig. 2.

**Projective fields.** The parameterization is guided by a so-called *projective field*, which is a vector field on $M$, where the vectors $v$ and $-v$ are identified for all $v \in T_pM$, $p \in M$. Thus, the vectors may change their sign without producing a discontinuous projective field. Note, that projective fields are a special case of $N$-RoSy fields for $N = 2$ as introduced by Palacios and Zhang [18].

The algorithm takes two projective fields as input and generates two scalar functions ($u$ and $v$), whose gradients match up with the input fields as well as possible. The coordinates $u$ and $v$ can be used as texture coordinates in order to map a pattern onto
the surface. If you are only interested in a stripe pattern, you could use only one input field and skip the computation of $v$.

**Construct an input field.** It is up to the user to construct an input field. A canonical choice is the field of minimum curvature: In each point, the corresponding vector points in direction of the (absolute) smaller principle curvature and has unit length. Using this field (together with the 90 degrees rotated field) as the input fields yields nearly curvature line parameterizations.

**The algorithm.** Starting from a given projective field, the algorithm first constructs a locally integrable field. Second, the surface is cut open to a topological disk and this field is integrated yielding a parameterization. Third, the parameterization is adapted such that the grid lines are connected across the cuts. Details are given in Sect. 4.

Special issues arise when the projective field has singularities. They are resolved by using branched covering spaces. The projective field naturally simplifies to a single vector field on the covering, and then standard Hodge-Helmholtz decomposition techniques are used to assure global integrability. Details are explained in Sect. 3.2.

3 Mathematical Setting

We use the theory of QuadCover’s 4-fold symmetric fields and apply it to the projective vector field setting with 2-way symmetry properties. We introduce the notion of projective vector fields and discuss consequences for the branched 2-fold covering spaces. We will describe our concepts in the smooth cast first, followed by the discretization for triangle meshes.

3.1 Parameterizations and Matchings

**Smooth case.** Given a smooth 2-manifold $M$ with charts $U_i \subset M$, $\sum_i U_i = M$. A parameterization is a collection of diffeomorphisms $f_i = (u_i, v_i)$ that map all charts into the parameter domains $f_i : U_i \rightarrow \Omega_i \subset \mathbb{R}^2$. One can now visualize the parameter lines on $M$ as the preimage under $f_i$ of the unit grid $\mathbb{N} \times \mathbb{R}$ ($u_i$ lines) and $\mathbb{R} \times \mathbb{N}$ ($v_i$ lines).
A **globally continuous stripe parameterization** consists of parameter functions \( f_i \) in the charts \( U_i \), such that the \( u_i \) lines (resp. \( v_i \) lines) coincide in all regions where two charts \( U_i, U_j \) overlap. Thus, the parameter lines of a stripe parameterization can be globally separated into \( u \)-lines and \( v \)-lines.

Given two guiding fields on the surface, we will only focus on computing the \( u \)-component from the first input field, as the same rules apply for computing \( v \) from the second field.

The transition functions between adjacent charts of a stripe parameterization satisfy two conditions: First, the gradients of \( u_i \) and \( u_j \) have to agree up to sign, because we do not distinguish \( u_i \) lines and \(-u_i\) lines on the parameterized surface. Thus, the gradients of the charts are related by

\[
\nabla u_i(p) = (-1)^{r_{ij}} \nabla u_j(p), \quad p \in U_i \cap U_j
\]

with a constant number \( r_{ij} \in \{0, 1\} \) on the intersection \( \Omega_i \cap \Omega_j \). We call the values \( r_{ij} \) **matchings** between charts \( U_i \) and \( U_j \).

Second, the values of \( u_i \) and \( u_j \) may differ only by integer values, since the \( u \) lines in the unit grid are invariant under translations by integer values.

Thus, we require the values of \( u \) in overlapping charts \( U_i \) and \( U_j \) to fulfill:

\[
u_j(p) = (-1)^{r_{ij}} u_i(p) + t_{ij}, \quad r_{ij} \in \{0, 1\}, \quad t_{ij} \in \mathbb{N}, \quad p \in U_i \cap U_j.
\]

**Discretization.** Each triangle of the mesh is considered as a chart. The transition function between two adjacent triangles is fully determined by the matching and the translation vector associated to their common edge, see (2). See Sect. 4.1 for details on how we compute the matching.

### 3.2 Projective Fields

A parameter function \( u \) can be characterized by its gradient field. In each chart, the gradient field \( \nabla u \) is a continuous vector field. At the transition between two charts \( U_i, U_j \), the sign of the vectors may flip depending on the matching. Thus, we cannot describe the derivatives of \( u \) as a globally defined vector field, but use **projective fields** which are invariant under sign flips.

**Definition 1.** Given a manifold \( M \) with charts \( U_i \) and matchings \( r_{ij} \). A **projective field** \( K \) on \( M \) is a collection of one vector field \( K_i \) in each chart \( U_i \), such that for all overlapping charts \( U_i \cap U_j \neq \emptyset \):

\[
K_j = (-1)^{r_{ij}} K_i.
\]

**Discretization.** The projective fields are piecewise constant on the triangles. Store one vector per triangle and the matching number on each edge. This fully defines a discrete projective field. An odd matching at any edge means that the vector in one adjacent triangle corresponds to the negated vector of the other triangle.
3.3 Branched Covering Spaces

We use the notion of branched covering surfaces for an equivalent description of projective fields. A projective field on the input surface can be regarded as a vector field on a covering surface. This allows us to apply standard vector field calculus to projective fields.

**Coverings.** First, recall some definitions on Riemann surfaces, see [5, 7, 14]. We will give an abstract definition of a covering and explain below how we actually construct one.

**Definition 2.** Let \( M \) be a Riemann surface. A **2-sheeted covering** \( M' \) of \( M \) is a Riemann surface with a local homeomorphism \( \pi : M' \to M \) with the property: For each point \( p \in M \), there exists a neighborhood \( U_p \) whose preimage \( \pi^{-1}(U_p) \) is the union of exactly two pairwise disjoint topological disks. Fig. 3, left shows a 2-sheeted covering.

We allow **branch points** \( p \) in our setting, where the preimage of a neighborhood of \( p \) is exactly one topological disk (instead of two), cp. Fig. 4, middle.

**Fig. 3.** From left to right: Trivial covering. / Patching two coverings together with matching \( r_{ij} = 1 \). / A projective field lifted to a vector field on the covering.

**Fig. 4.** Left: Stripe parameterization with branch point. The isolines of the \( u \) function and its gradient vectors are drawn. Middle: The same parameter function on the 2-sheeted covering (the covering surface is not embedded, it has self-intersections). Right: Branch point on a parameterized tube object.
**Construction.** We construct a covering of $M$ as follows: From each chart $U_i$, make two copies (layers) and name them $U_{i,0}'$ and $U_{i,1}'$. Let $\pi_i : U_{i,0}' \cup U_{i,1}' \rightarrow U_i$ be the operator which projects the copies back to $U_i$ and $\tau_{i,0} : U_i \rightarrow U_{i,0}'$, $\tau_{i,1} : U_i \rightarrow U_{i,1}'$ the inverse maps. The two layers $U_{i,0}' \cup U_{i,1}'$ together with $\pi_i$ is called the 2-sheeted trivial covering of the chart $U_i$ (Fig. 3, left).

In the next step, we glue these layers at the overlaps of the adjacent charts together. For each pair of charts the layers can be glued in two different ways. The matchings $r_{ij}$ define how the layers are identified.

**Definition 3.** A covering surface induced by matchings $r_{ij}$ is uniquely defined by the following construction:

Let $(U_i', \pi_i)$ be 2-sheeted trivial coverings of the charts $U_i$. The covering surface is given as the union of all $U_i'$ where the following points are identified: In each two overlapping charts $U_i, U_j$, identify all points $\tau_{i,0}(p)$ with $\tau_{j,r_{ij}}(p)$ and $\tau_{i,1}(p)$ with $\tau_{j,1-r_{ij}}(p)$, $p \in U_i \cap U_j$ (see Fig. 3, middle).

Since the trivial coverings of charts have no branch points and the charts cover the surface, we cannot construct any branch points this way. We allow branch points by removing single points from the surface. Depending on the matchings we obtain a branch point there as shown in Fig. 3.

**Discretization.** In the discrete setting, branch points are located at vertices. On a 2-sheeted covering they occur when the sum of all matchings of incident edges is odd. This means starting somewhere in the neighborhood of $v$ and walking once around the vertex ends on a different layer in the covering than the start point.

### 3.4 Vector Fields on Covering Spaces

Projective fields can be described as vector fields on a covering surface. This result allows us to apply the classical vector field theory to projective fields.

A projective field $K$ on $M$ with matchings $r_{ij}$ canonically lifts to a vector field $K'$ on the covering induced by $r_{ij}$. In each chart $U_i$, define the vectors on its trivial covering as follows: For all $p \in U_{i,0}'$ set $K'(p) := K_i(\pi_i(p))$ and for $p \in U_{i,1}'$ set $K(p) := -K_i(\pi_i(p))$, see Fig. 3, third image.

The result is a globally well defined vector field $K'$ on $M'$, since the layers of the covering are connected in the same way as the vector fields permute when another chart is chosen.

**Definition 4.** Let $M$ be a manifold with matchings $r_{ij}$ and $M'$ the induced covering. A projective field lifted to a vector field $K$ on $M'$ is called a covering field of $M$.

### 4 Stripe Parameterizer Algorithm

In this section we describe the main extensions and simplifications which have been made to QuadCover to yield the stripe parameterizer. An important difference is the use of projective vector fields instead of frame fields.