Computational Topology for Molecular Animation

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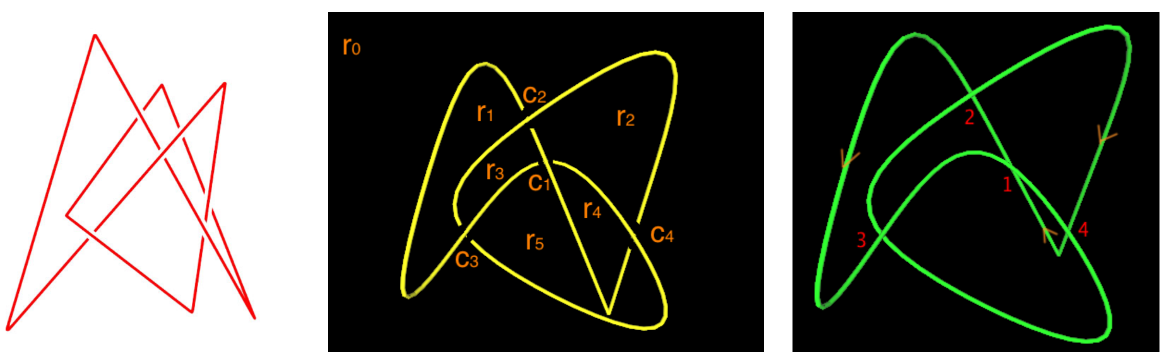
Abstract: Scientific visualization typically depends upon piecewise linear (PL) geometry. Dynamic visualization of molecular simulations is often discussed, informally, as "molecular animation". Some of these molecules are mathematically modeled as knots and computationally instantiated as splines. Questions arise of topological consistency between the geometry and its PL approximation, with considerable existing literature on *static* cases. This work warns of topological inconsistencies that could elude the attention of the viewer in the *dynamic* case.

Keywords: Knot, isotopy, visualization, molecular simulation.

1 Introduction

The preservation of topological characteristics during approximation for graphics is of contemporary interest [1]. Applications to dynamic visualization in molecular simulations in a high performance computing (HPC) environment have appeared [2, Proposition 5.2], as changes of embedding have chemical significance. A fundamental question is "When do two curves have the same embedding in $\mathbb{R}^3$?" For knots, the question becomes ambient isotopic equivalence. For molecular simulations, it is important that the synchronous animation does not mislead the viewer. This work presents a case where the viewer might miss a subtle change of embedding.

The image of Figure 1(a) shows a PL graphics approximation for the associated Bézier curve of Figure 1(b), where these two curves are ambient isotopic. Figure 1(c) is a different knot, the unknot, generated by perturbing only one vertex.



(a) Stick Knot (b) Isotopic Knot (c) Unknot (after perturbation)

Figure 1: Comparing the Topological Embeddings of Curves.

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2 The Experimental Example

The standard definition for a Bézier curve [4] is expressed by $\mathcal{B}(t)$, of degree n with control points $P_m \in \mathbb{R}^3$ with

$$\mathcal{B}(t) = \sum_{m=0}^{n} \binom{n}{m} t^m (1-t)^{n-m} P_m, t \in [0,1],$$

Since close approximation often leads to isotopic equivalence, the iterative addition of midpoints to each edge of Figure 1(a)was experimentally shown to reduce the distance between the control polygon and its Bézier curve[1]. The computational advantage is retention of the original edges, as opposed to subdivision [4] increasing the number of edges exponentially. Figure 1(b) was generated from Figure 1(a) by this midpoint insertion technique.

The original curve data was captured as the collection of control points, denoted as $\mathcal{P}_1$,

$$(1.30, -3.33, -2.50), (-1.38, 4.68, 0.91), (-3.29, -4.05, 2.68), (-0.12, 2.77, -2.46),$$
$$(3.91, -4.53, 1.23), (-3.94, -0.44, -0.98), (3.22, 4.30, 2.11).(1.30, -3.33, -2.50).$$

Denote the first vertex as v_0 and translate v_0 to $(1.9817, -1.7646, -4.5897)$. The first geometric verification is that $\mathcal{P}_1$ is simple, which follows easily from standard line segment intersection tests over the *original* edges. Similarly, it is shown that the translation of v_0 produces no self-intersections along the entire translation path, proving that $\mathcal{P}_1$ and its perturbation are ambient isotopic. In the planar projection shown in Figure 1(a) there are a total of 6 self-intersections, but inspection of the z-coordinates of these projected planar intersections reveals 3 consecutive overcrossings, so that 2 of these can be eliminated with Reidemeister moves [3] to establish knot type 4_1. A similar static planar intersection analysis was done for Figures 1(b) and 1(c), but the simplex method was used because of the increased geometric complexity. Again, the crossings were analyzed to posit that Figure 1(b) was also 4_1 – corroborated by computation of the Alexander polynomial as $1 - 3t + t^2$ (The annotations indicate the input crossings and regions.) For Figure 1(c), the intersection analysis showed that the crossings labeled as '1' and '2' are under crossings, while '3' and '4' are over crossings, to confirm that this is the unknot. Thus, the perturbed PL knot 4_1 is no longer isotopically equivalent to the corresponding perturbed Bézier curve of the unknot.

3 Conclusion

For synchronous visualizations of writhing molecules, a cautionary example is presented of different knot types between a Bézier curve and its rendering. The example was discovered by visual experiments and then formally verified by computational geometry algorithms and knot theory.

References

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[1]This convergence conjecture has been formally proven, but that result is beyond the scope of this short abstract.