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Topological subtleties for molecular movies

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ABSTRACT

Synchronous movies permit visual analysis of shape perturbation during molecular simulations. The molecule is conceptualized as a knot and modeled as a spline curve. As the molecule writhes, the graphics approximation in each frame should display an ambient isotopic image of the perturbing spline. These graphics approximations raise subtleties for correctly rendering the embedding. A cautionary example was discovered through visualization experiments and the relevant characteristics are formally proved.

1. Introduction

For a molecular movie, a piecewise linear (PL) curve is created as an ambient isotopic approximation of an initial static spline. The frames of the movie are then based upon this PL approximation. Topological artifacts could be introduced. Consider the spline curve **c** depicted in Fig. 1(a) and its PL approximation, **k** of Fig. 1(b). Both **c** and **k** are the knot 4_1 and are defined by the same set of vertices, $\mathcal{P}$. In this example, a vertex of $\mathcal{P}$ is translated to produce $\mathbf{k}^*$, which is still 4_1, as shown in Fig. 1(c). However, the spline defined by these perturbed vertices is the unknot $\mathbf{c}^*$ of Fig. 1(d). A molecular movie using the incorrect embedding of Fig. 1(c) could mislead the viewer.[2]

During development of computer animations, attention to the appropriate embedding can be overlooked. For performance reasons, it is common to assume that an initial PL approximation suffices for all subsequent movements of the spline. Sufficient conditions have been given [14] where this prevails, but we provide a cautionary example outside those limits. Particularly poignant about this example is that the change of

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[2] The images of Figs. 1(c) and 1(d) were taken under slightly different projections than those of Figs. 1(a) and 1(b) to more clearly show the embeddings.

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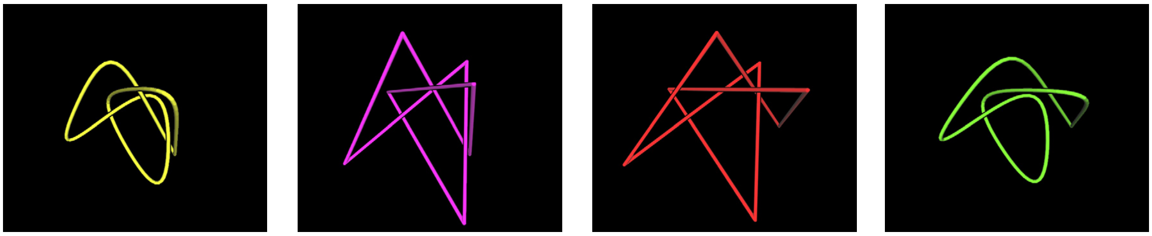

(a) Spline 4_1, $\mathbf{c}$ (b) PL 4_1, $\mathbf{k}$ (c) PL 4_1, $\mathbf{k}^*$ (d) Spline Unknot $\mathbf{c}^*$

Fig. 1. Comparing embedded spline curves to their approximated images.

embedding does not occur for the PL approximations, only the splines, so that the viewer could be misled, since only the PL approximations are rendered.

2. Related work

The term ‘molecular movies’ includes “... molecular animations ... ” [22]. A contemporary treatment of knots and molecules [26] provided motivation for the visualization software [21] used here to explore topologically correct computer animation of knots.

The preservation of topological characteristics in computational applications is of contemporary interest [1–3,8,9,12–15,17,20]. Sufficient conditions for a homeomorphism between a Bézier curve and its control polygon have been studied [24], while topological differences have also been shown [5,18,25]. Sufficient conditions were given to insure that perturbations of the control points maintain isotopic equivalence of the perturbed splines [4]. There is an example of a PL structure that becomes self-intersecting while the associated Bézier curve remains simple [7].

The standard definition for a Bézier curve [25] of degree n is expressed by $\mathcal{B}(t)$, with control points $P_m \in \mathbb{R}^3$ with

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

The curve formed by PL interpolation on $\mathcal{P} = \{P_0, P_1, \ldots, P_n\}$ is called the *control polygon*.

3. The defining data for the example

Consider the points $v_0, v_1, \ldots, v_7$, listed cyclically as (with $v_7 = v_0$):

$$(1.3076, -3.3320, -2.5072), (-1.3841, 4.6826, 0.9135), (-3.2983, -4.0567, 2.6862),$$
$$(-0.1233, 2.7683, -2.4636), (3.9080, -4.5334, 1.2264), (-3.9360, -0.4383, -0.9834),$$
$$(3.2182, 4.2961, 2.1125).$$

Let $\mathcal{P} = \{v_0, v_1, \ldots, v_7\}$ be the set of control points defining a closed Bézier curve. We iteratively inserted new control points as midpoints of this initial control polygon and observed that the generated Bézier curves approached the initial control polygon. Note that this process preserves the embedding of the initial control polygon. This strategy was motivated by experimental evidence that low degree curves were unlikely to display the expected artifact, while also wishing to minimize the number of relevant edges. Fig. 1(a) shows the 112 degree Bézier curve created after 4 iterations of inserting midpoints, with the associated control point, $\mathbf{k}$ shown in Fig. 1(b).