Crystallizing Topology in Molecular Visualizations

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Abstract

The integration of evocative images with analytic perspectives can facilitate scientific discovery. The images can prompt scientists to become more deeply engaged in the interpretive process as a stimulus to further creative insight.

1 Artistic Stimulus of Chemical Discovery

Molecular topology and function are closely related in ways that are not yet fully understood. Humans often infer these topological characteristics and relationships from images. Aesthetically pleasing graphics can facilitate that understanding. The stick model of $\mathbf{CO}_2$ is shown as Figure 1. However, when special lighting effects and crystals were added in Figure 2 to distinguish between the energetic and frozen states, scientists gained significantly more understanding of carbon freezing by an interpolative animation paired with interpretive algorithms. Creative stimulus came from a chemist observing the crystal changes of snow falling into a river.

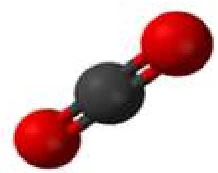
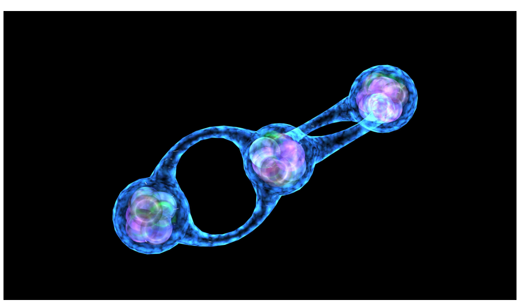
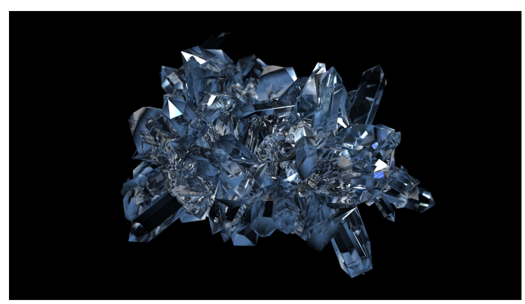


Figure 1 : *Ball & stick*



(a)



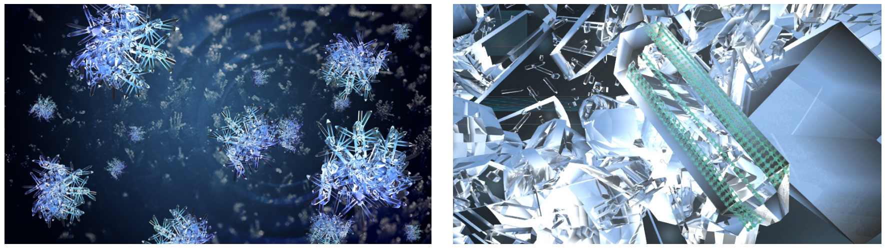
(b)

Figure 2 : *Energetic and Frozen States*

T. Hunter pioneered the depicted high-resolution 3D digital animation techniques, inclusive of scaling to 9600 x 1080 – a resolution previously unattained in an HD format. The animation has been effective at generating scientific hypotheses and stimulating popular curiosity into complex petro-chemistry[1].

Figure 2(a) was the first frame in an animation ending with Figure 2(b), for a process known as carbon freezing. Scientific insight into carbon freezing was greatly enhanced by an interpolative animation between these frames, with story board elements shown in Figure 3. The visual observation, captured in Figure 3(a), was that as the snow crystals fell and landed in a river, they did not melt but were carried away by the flow. This triggered the insight that if $\mathbf{CO}_2$ molecules were frozen to crystals within a stream of liquid $\mathbf{CO}_2$, then the crystals would emerge from an enriched and purified gaseous environment, as depicted in Figure 3(b).

[1]This work was conducted under a proprietary agreement between T. Hunter and ExxonMobil Corporation and this is the first summary approved for public release.



(a) (b)

Figure 3 : *Story Board: Snow Crystals in Flowing River and* $\mathbf{CO}_2$ *Crystals Forming*

2 Related Work

The rich history of the role of knots as mathematical models for molecules is nicely summarized and extended into beautiful contemporary computer graphics and animations [13]. Knot theory is a specialty within topology and the effectiveness of topology as a powerful abstraction for visualization resonates through the "Topology in Visualization Workshops" [3, 10]. The preservation of topology in visualization is also explored under *"mathematically precise visualization* [4] and *"verifiable visualizations"* [5]:

> that will consider both the errors of the individual visualization component within the scientific pipeline and the interaction between and interpretation of the accumulated errors generated in the computational pipeline, including the visualization component.

Topological differences between Bézier curves and their control polygons regarding self-intersections have been presented [9] with emphasis upon subdivision [11]. Theory for ambient isotopic equivalence of splines [1] under perturbations has appeared. The value of computational tools in "aesthetic engineering" [15] has been realized in knot sculptures [14].

3 Topological Theory for Changes in Shape

Section 1 presents the value of aesthetically pleasing images to facilitate understanding of carbon freezing. Dynamic changes in the form of $\mathbf{CO}_2$ molecules were depicted through human creativity. Visualizing dynamic changes for other molecules will rely upon developing formal abstractions of those changes in form. Supportive graphics have prompted discoveries in computational topology for these formalisms.

Relevant topological characteristics are now informally explained. Splines were used as the geometric data in the animation frames described in Secion 1 and there are topological subtleties to consider for spline approximation by the control structure for graphics display. One topological subtlety [2] is shown in Figures 4. The spline curve and the PL structure have different embeddings, as the PL curve is the trefoil knot[2], while the spline curve is unknotted [7].

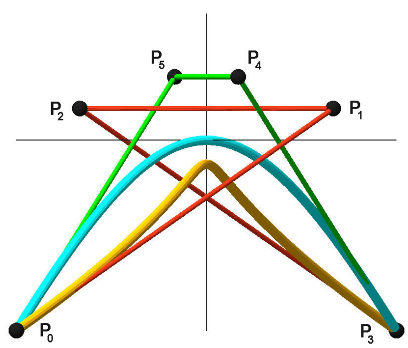


Figure 4 : *Knot Graphics*

Denote by **c** the closed, composite cubic Bézier curve[3] with control points, $P_0, P_1, \ldots P_5, P_0$, respectively listed as: (-6, -6, 12), (4, 1, -1), (-4, 1, 1), (6, -6, -12), (1, 2, 4), (-1, 2, -4), as shown in Figure 4. Curve **c** is the unknot but the control poly-

[2] A trefoil is the knot with three alternating crossings.

[3] Bézier curves are a class of spline curves.

gon, denoted as K is a trefoil [2]. The symmetry of K results in two superfluous [7] undercrossings: $[P_2, P_3]$ under $[P_5, P_0]$ and $[P_2, P_3]$ under $[P_0, P_1]$. One co-author had advocated for this symmetry to make for more aesthetically pleasing images. Another author countered that these extra crossings would complicate the mathematical analyses needed to ensure a sufficiently fine approximation to produce the correct approximated shape. However, hat analysis was simplified by the symmetry about the vertical axis, which more than compensated for the extra crossings. These visual experiments led to a formal theorem that ensures equivalence of knot type under subdivision for Bézier curves up to degree 3, as a theoretical foundation for faithful graphics display [8].

4 Topology Visualizing Tool for Mathematical Discovery

The value of these spline visualizations for discovery in computational topology led to the development of additional software and further mathematical discoveries, as now described. The visually expressive models of $\mathbf{CO_2}$ presented remain too complex for initial mathematical study for the fundamental topological relations between a spline and its PL approximation by subdivision [11]. The software *Visualize-Knots-Curve-Tool* was implemented to aid that mathematical discovery. The Knot_Plot site [12] provides data sets for PL knots with edges all having the same length, where a representative example is shown in Figure 5. After viewing many such examples, it was conjectured that the associated Bézier curve would always be simple. As this conjecture was subjected to detailed mathematical analysis, a counterexample was developed [6]. This visualization tool for the topologist is similar to sketches for a painter.

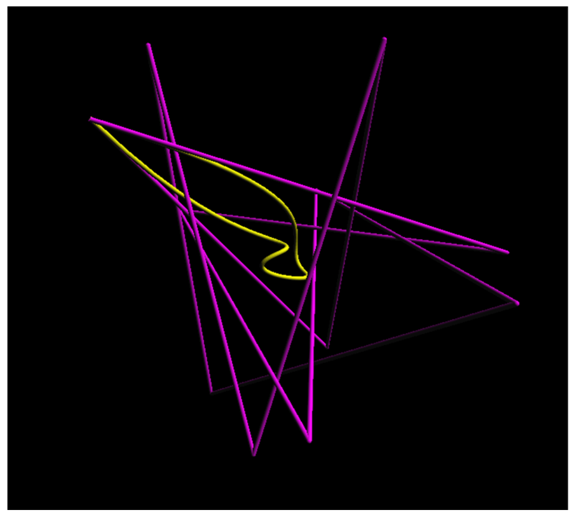


Figure 5 : *Math Model*

To scale our topological analyses, the authors have created software for building simplified geometric models of large protein molecules, with capabilities for graphics display and animation to study how to preserve desired topological properties. One of our large protein images is shown in Figure 6, where many crossings are readily visible. With knots serving as molecular abstractions, it is worth noting that the complexity of knot characterization often increases exponentially in the number of crossings, arguing for computational tools like *Visualize-Knots-Curve-Tool* for as few as 5 or 6 crossings.

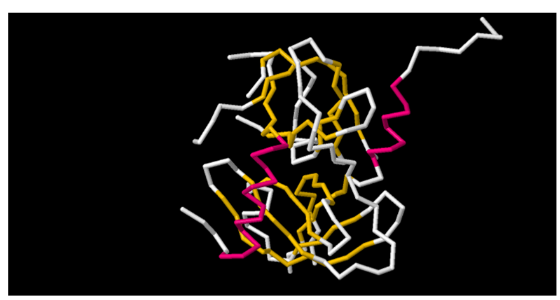


Figure 6 : *Protein Model*

5 Conclusions and Future Directions

Topological methods are emerging as powerful tools in visualization for molecular models. The effectiveness of topology is further enhanced by additional focus on the aesthetics of the images presented, which not only produces more artistic images, but also accelerates progress in scientific discovery. It remains crucial to verify visual experiments with rigorous analysis lest appealing conjectures are erroneously accepted from extensive data that happens to miss critical pathologies.

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