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# Through a *New* Looking Glass*: Mathematically Precise Visualization

*By Kirk E. Jordan, Robert M. Kirby, Claudio Silva, and Thomas J. Peters*

Alice gazes through her looking glass at a perplexing world that confuses her [3], as vividly depicted in the recently released 3D movie *Alice in Wonderland*. Scientists, peering through their new looking glass of scientific visualization, derive illuminating insights from otherwise impenetrable petabytes of simulation data.

Scientific visualization, however, presents some mathematical challenges of which the general mathematical community should be aware. Most important is a delicate computational balance that must be attained between exact topological properties and their computational approximations [9]. The driving imperative is to prevent visual artifacts that would cloud the scientists' interpretations, as happened to a confused Alice. The story of the integration of geometric modeling with computational fluid dynamics and other simulations offers guidance for the solution of similar mathematical problems in scientific visualization.

The final stage in the scientific method is the communication of results. This stage is often as important as hypothesis formulation or experimental conclusions. Scientific visualization encompasses both the exploration and the explanation of scientific results. Issues of complexity and precision abound. In contrast to Alice's world, scientific visualization should produce imagery that illuminates computational experiments. Much as 3D stereovision enriches the movie-viewing experience, mathematically precise visualization will enrich scientific discovery.

Scientific visualization relies on many of the same mathematical (numerical) tools used to build simulations, requiring that visualization scientists ask questions concerning model validation and numerical verification. The images in Figure 1, with their increasingly complex geometry and topology, illustrate what's required: Figure 1(a) has obviously discernible separation at its crossings; as such separations become progressively finer in (b) and (c), increasingly sophisticated approximation algorithms and numerical analyses are needed to guarantee graphics that will support unambiguous visual interpretation of the appropriate topology.

The preservation of topology is one property explored in "verifiable visualizations" [10], which

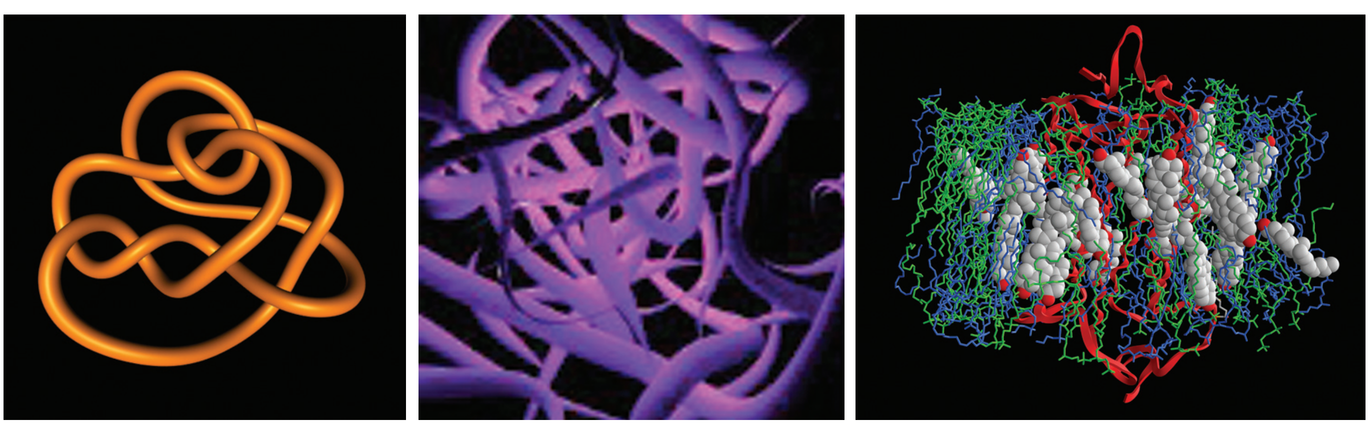
"will consider both the errors of the individual visualization component within the scientific pipeline and the interaction between and interpretation of the accumulated errors generated in the computational pipeline, including the visualization component."

Strict error analysis and verification have been the norm in simulation science, but not in scientific visualization. Quantification of approximation errors is the critical component of verifiable visualization. Every visualization proceeds from an approximated model. It is important to understand not only the original errors of approximation in a model, but also how those errors can degrade engineering analyses that use the model.

Because approximated geometric models are used as input for sensitive engineering analyses of computational fluid dynamics, computational electromagnetics, and finite element analysis [4], the computer-aided geometric design community has long been extremely attentive to the magnitude of model approximation errors. Early methods were often purely *ad hoc* and consequently resulted in significant direct economic losses and lost productivity [2]. Some guiding mathematical abstractions have been proposed [6] (see Table 1); the values are not exact, but indicate the relative accuracy needed for different applications. The key point is that there is no one universal tolerance. The question of a computing tolerance is meaningful only in the context of a particular application.

The essence of the message from CAGD is that differing engineering analyses will typically require models created at differing levels of accuracy and precision [4]. In the much less mature field of visualization, we have opportunities to learn from and avoid those early CAGD mistakes [15]. Contemporary visualization presents challenges in scale, from the pharmacological design of macromolecules to the engineering fabrication of nanomechanisms, that extend far beyond past CAGD practice. These new challenges provide excellent opportunities for engagement by the applied mathematics community, across academia and industry.

*With apologies to Lewis Carroll [3].



**(a)** **(b)** **(c)**

**Figure 1.** *(a) Unknot [18], (b) complex knot [18], (c) molecular model [1].*

In considering how to proceed, we can find some guidance by examining responses in the CAGD literature. One spline surface intersection algorithm [8] incorporates precise determination of the starting points of intersection curves [17] and a topological sorting of intersection components to prove rigorous error bounds on the output intersection set. A straightforward application of Taylor's method converts those parametric domain error bounds into error bounds in $\mathbb{R}^3$, which is the co-domain of each spline function [16]. This brief summary suggests the fundamental importance of the mathematics of splines, numerical analysis, topology, and real analysis in the development of responsive surface intersection algorithms. Similar mathematical breadth will be required for the algorithms needed to achieve precise scientific visualization.

| Application | Minimum Precision |
|---|---|
| Visualization | $10^{-2}$ |
| Computational Fluid Dynamics | $10^{-3}$ |
| Multidisciplinary Design Optimization | $10^{-4}$ |
| Computational Electromagnetics | $10^{-4}$ |
| Computational Optics | $10^{-7}$ |

**Table 1.** *Precision guidelines for differing applications.*

Concern for accuracy in computational fluid dynamics was one of the problems that motivated the development of Table 1 [4]. The disparity between many contemporary visualizations and the CFD results visualized prompted the comment that CFD could stand equally well for "colorful faulty dynamics" [10]. In this article for the SIAM community, we present a visualization example from CFD, intended to be representative of a wide range of relevant disciplines, echoing the CAGD experience. The CFD visualization example typifies mathematical issues in verifiable visualization. Appropriate precision permits faithful representation of essential model characteristics. Following this introductory CFD example, this theme is continued with examples from recent research on preserving topological properties during visualization.

Our representative example, depicted in Figure 2, illustrates potentially incorrect conclusions that can be drawn from an ill-suited visualization. Solving the advection term in synthetic fluid flow in a Lagrangian fashion by bilinear interpolation is a common but flawed method for evaluating the velocity field: "Although this approach is unconditionally stable even with relatively long time-stepping, it is subject to numerical diffusion due to interpolation."[10] The result, as shown in Figure 2, is a visual smearing artifact that is due entirely to the algorithm and not related to the physical process.

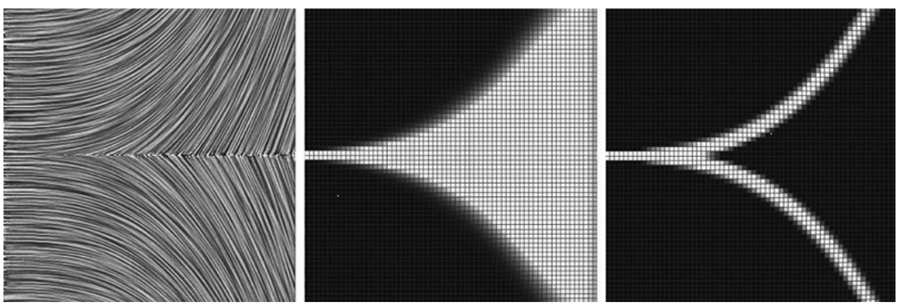


**Figure 2.** *Visualization of a synthetic flow exhibiting splitting behavior. Left, dense texture visualization in GPUFLIC [11]. Middle, dye advection visualization by the semi-Lagrangian texture advection scheme. The pattern appears to be divergent and diffusive. Right, accurate visualization by the physically based control volume dye advection scheme.*

Early work on the verification of widely used visualization algorithms has generated surprises. For instance, recent results of Etiene et al. [5] on the verification of topology determined by isosurface extraction techniques reveal either minor conceptual flaws or incorrect implementations of several existing codes. This group used techniques from digital topology and stratified Morse theory to develop systematic mechanisms for testing the correctness of isosurface codes. These preliminary results provide initial diagnostic information. As isosurface extraction is foundational for many visualization techniques, the results suggest the need for greater emphasis on the use of a rigorous verification methodology for visualization tools. Figure 3 summarizes some of the errors that would impede correct visual interpretation.

Analysis of the region shown in detail in Figure 3(a) led to the conclusion that the output surface does not have the "closed-disc property"; the result is a topological artifact. In Figure 3(b), the middle image shows the expected output. The image on the left differs topologically from what was expected; the difference was traced to a conceptual issue. An orientation mismatch was not foreseen by the creators of this isosurface algorithm. The image on the right shows a trilinear surface that was constructed as part of the diagnostic process [5]. In Figure 3(c), the two models were both found to have the correct topology, but further analysis exposed geometric anomalies, the result of a coding error, in the image on the left.

Underscoring the timeliness of this topic, an article on mathematics for special effects appeared while we were preparing this article; that article additionally discussed applications to dynamic visualization for surgical simulations [14]. These concurrent articles share an emphasis on CFD and topology extraction from meshes [13], but differ in that the other article treats isosurfaces as applications of level set methods.

Scientific visualization also has considerations that extend beyond any mathematical theorem. Certainly, convergence rates are a common concern. Visualization also integrates human interaction that cannot be fully captured mathematically. Effects of errors in visualization can be as benign as things that "look wrong" (often discussed informally as the "eyeball metric"), but they can also be drastic, as in the case of researchers who draw incorrect conclusions or make incorrect deductions from their data. Visualization scientists will sometimes forgo further mathematical refinements in favor of more pragmatic interactivity when a quick, rough answer becomes a compelling catalyst for more penetrating questions.

In summary, the message to the SIAM community is that visualization science has been enriched by the mathematics of numerical analysis, splines, topology, and level sets *and* that the field is rich in opportunities for further mathematical contributions. A central issue is the integration of appropriate mathematics in visualization algorithms to facilitate enlightening abstractions from massive volumes of simulation data.

## Acknowledgments

The authors express their appreciation to David R. Ferguson and Thomas A. Grandine for their helpful comments and insightful observations. Figures 1(a) and 1(b) are publicly available [18]; the images in Figure 1(c) [1] and Figure 2 [12] are used with permission.

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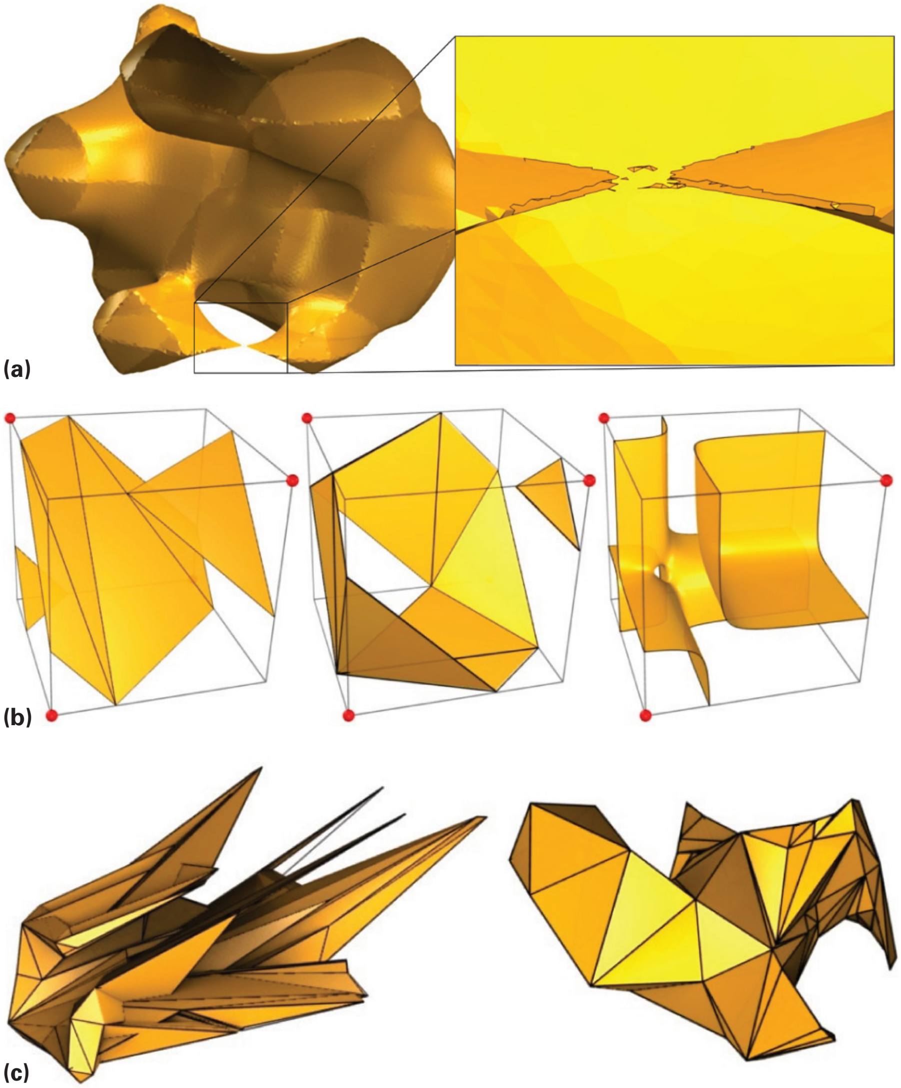


**Figure 3.** *Summary of errors discovered [5]. (a) A topological artifact. (b) The lefthand image has incorrect topology; the middle image has the correct topology, and the righthand image shows a surface that was created as a step in the topology-verification process. (c) The righthand image is both topologically and geometrically correct; there are geometric flaws in the lefthand image.*


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*Kirk E. Jordan is the Emerging Solutions Executive, Computational Science Center, at the IBM T.J Watson Research Center. Robert M. Kirby and Claudio Silva are associate professors of computing at the University of Utah. Thomas J. Peters is a professor of computer science and mathematics at the University of Connecticut.*