

Visualization of Topological Defects in Nematic Liquid Crystals Using Streamtubes, Streamsurfaces and Ellipsoids

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Researchers in computational condensed matter physics deal with complex data sets consisting of time varying 3D tensor, vector, and scalar quantities. Particularly, in the research of topological defects in nematic liquid crystals (LC) displaying the results of the computer simulation of molecular dynamics presents a challenge. Combining existing immersive and interactive visualization methods we developed new methods that attempt to provide a clear, efficient, and intuitive way to visualize and explore LC data. In addition, the visualization of the data has presented us with a novel method of obtaining the locations of the topological defects present in a liquid crystal system.

METHODS

Our visualization approach is applied to the results of molecular dynamics simulations of Billeter et al. [2]. These data take the form of a 2^{nd} order 3D tensor field describing the orientation of each LC molecule. We then sample this field using a cubic B-Spline as a sampling kernel or point spread function. We vary both the radius of the kernel and the dimensions of the resulting field. In order to clarify the subsequent features of the resampled field we introduced padding. The original LC sample is topologically equivalent to a hypertorus because of periodic boundary conditions. We extend the original dimensions of the field by reproducing a portion of the data in every direction. This way, the features that wrap from one side of the data to the next appear to be continuously repeating thus allowing for better spatial coherence.

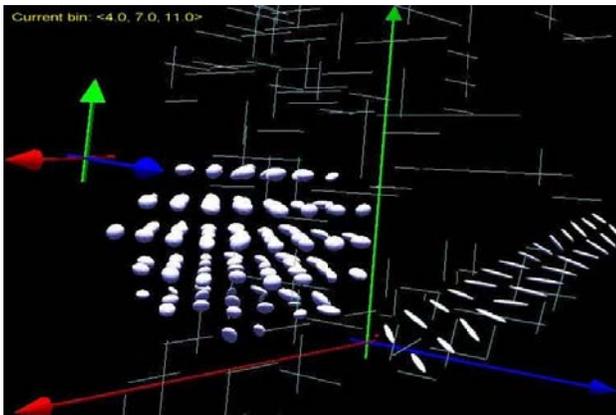


Figure 1. Selected area of groups of molecules (~30) on the left represents tensor valued order parameters for each group. Partial layer on the right represents bidirectional vector valued average orientation of molecules within those groups. In addition to the set of world coordinate axis, the miniature axis cursor follows a tracked 6 degree-of-freedom device by showing orientation of the world during navigation and displaying the cursor's coordinates (top left).

We implement two methods to visualize the resulting resampled, padded 2^{nd} order 3D tensor field. The first method uses an array of ellipsoids where the shape of each ellipsoid represents one tensor value [3]. The average orientation of molecules in each group (the primary axis of the scaled ellipsoids) is visualized as an elongated 'cigar' to represent the bidirectional vector quantity. Utilization of the CAVE, a virtual reality environment [4], allows application of highly interactive methods for navigating, exploring and

understanding the data model presented.

We implemented a set of interaction techniques such as navigation, dynamic selection of areas and layers to aid in detailed exploration of data. We supplemented these techniques with positional and orientational cues [Figure 1].

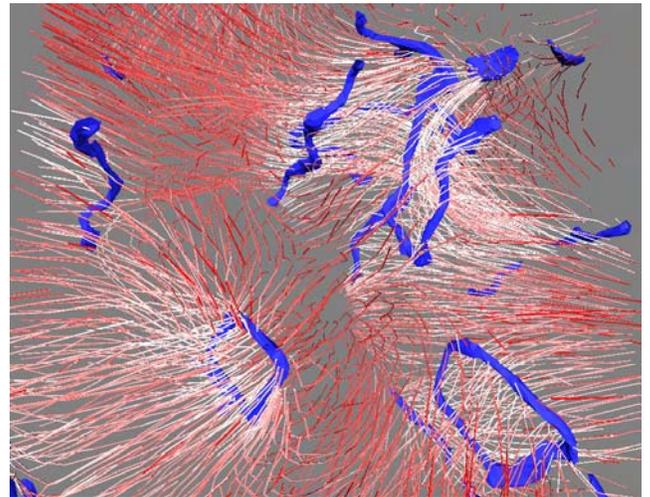


Figure 2. The visualization of the resulting data includes the stream tubes (red tubes representing the directions of higher linear anisotropy values which are the average orientations of the molecules along those paths) and isosurfaces (blue hollow tubes representing areas of constant low linear anisotropy values which are the areas where defects occur). The meshes were generated in the OpenInventor format and were loaded in a scene viewer that allowed for basic mouse and keyboard manipulations.

The second method utilizes the Westin et al. anisotropy metrics [5] to measure the level of linear and planar anisotropy and isotropy in the resampled tensor data. Once these measures are known, the data is integrated to find the streamlines of constant linear anisotropy values [6]. These streamlines represent the average molecular orientation in regions outside the topological defects. The defects themselves correspond to regions of low linear anisotropy which can be visualized by plotting the isosurfaces of constant low isotropy values resulting in the closed surfaces topologically equivalent to a n -torus ($n > 0$). The isotropy value chosen is varied to produce the desired visualization effect as the isotropy value changes the diameter of the tube comprising the surface. [Figure 2].

RESULTS

The data used for the visualization is a snapshot of the liquid crystal system at a time step in the simulation where the defects are well separated from each other [2]. The system consists of ~64K molecules each represented by a 2^{nd} order 3D tensor at a particular location. Therefore, for each molecule we have nine (9) measures and so the data is stored in ASCII or binary file with 9 floats per line per molecule.

The virtual reality visualization method was geared towards visualizing the tensor field information for more intuitive and

interactive analysis. The availability of interaction tools in the virtual environment reportedly allowed the users to quickly pick the most comfortable settings to view the tensor data. By allowing the user to physically walk through the virtual structure, all areas of the model were available for immediate inspection in the virtual space [4] using various navigation interactors.

Additional depth cues such as lighting, coordinate axis, miniature coordinate axis cursor showing world orientation, as well as displaying current cursor position helped the users keep track of their orientation with respect to the model in the virtual environment.

The second method involved the visualization of the resulting data that could be interpreted by the scientists as topological defects and the behavior of the LC system around their vicinity. The streamtubes show the molecular orientation around the cores of the topological defects, providing insight into the nature of the defects. The isosurfaces of low linear anisotropy formed closed loops (representing defect loops) with streamtubes 'flowing' through the plane of the rings thus formed. Such features appeared to be consistent with the defect findings using previous approaches by the LC researchers [2].

Because the 3D features obtained by analyzing tensor data so closely matched the expected physical features of LC data, the LC researchers have found a new way of finding defects which is less computationally costly and is based directly on the behavior of the tensor field. In comparison to the CAVE visualization, the method of sampling the tensor field and extracting Westin metrics combines both finding and visualization of defects in the way that was never done before. For the first time the researchers were able to correlate the appearance of defects and the tensor field behavior around the areas where the defects occur.

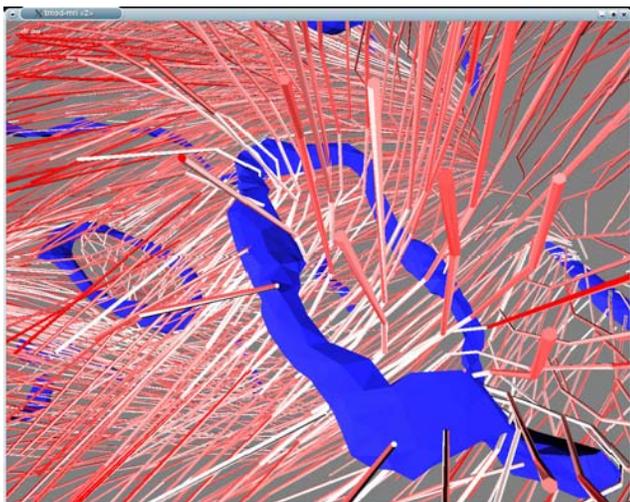


Figure 3. This collection of blue-colored isosurfaces formed closed loops (topological defects). The streamtubes flowing through and around them lie in the directions of higher linear anisotropy values above a certain threshold.

CONCLUSIONS

As reported by the users and in light of further advances in LC defect visualization, the virtual reality method has proved to be a

good way to visualize and explore existing data. It allows for extensible interaction methods and provides a novel interface to molecular data exploration. Specifically to LC research, this approach falls short of displaying clear structures and patterns within the data in the context of topological defects. If further developed and combined with the Westin metrics method it can potentially emerge as a powerful virtual reality molecular data visualization tool.

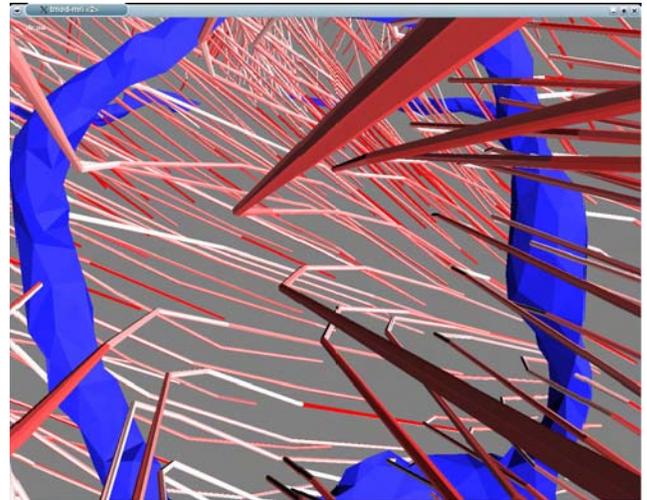


Figure 4. The closeup of the loop structure (blue) reveals the details of the behavior of the system around the vicinity of the defect (the core). Because the streamtubes (red) are appropriately spaced out, the user can zoom in and effectively explore the cores of the easily identifiable defects.

The power of Westin metrics method is exhibited in the fact that even the most trivial exploration of the meshes generated presented a novel method for identifying the defect patterns. The defect finding was performed using a drastically different approach and results matched with previous calculations using geometric methods[1]. More sophisticated depth cues (stereo, lighting, texturing) can improve users' ability to investigate important patterns in the data.

Some of the challenges that lie ahead are visualization of time-varying data, improving interactivity, searching for other physically relevant features of the resampled tensor field.

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