Exploring Defects in Nematic Liquid Crystals

Ketan Mehta*, Matthew Lee† and T.J Jankun-Kelly*
Mississippi State University

Figure 1: Liquid Crystal Data Explorer - Composite view (left) and Detail view (right)

ABSTRACT

Visualization of temporal and spatial tensor data is a challenging task due to the large amount of multi-dimensional data. In most of the visualization, scientists are interested in finding certain defects, anomalies, or correlations while exploring data. Hence, visualization requires efficient exploration and representation techniques. In order to use the nematic liquid crystal (NLC) as a biosensor, scientists need to study and explore simulations for understanding the relationship between topological defects and the biological specimen.

To solve the above problem, we merge scientific and information visualization techniques to create a controlled exploration environment. System enables a user to filter and explore NLC data sets for orientation defects. We introduce a three level visualization approach for exploring tensor data sets using timeline, parallel coordinate, and glyph based visualization. Visualization helps in reducing unnecessary data at each stage and focus on the relevant ones. This abstract discusses the goal, approach and various research issues found in the design of the NLC data visualization system.

1 RELATED WORK

Tensor data is encountered in the study of various scientific and analytical tasks and used across the engineering domains like medical imaging [2], computation fluid flow analysis, and mechanics. Current research focuses on finding new techniques for efficient glyph generation, topology extraction, or tensor decomposition [1]. Most tensor visualization techniques decompose the second-order tensor

matrix into three independent eigen value and vector sets forming the basis of the superquadric or ellipsoidal glyph [4] [7]. Glyph rendering has been augmented by various perceptual cues like texture, color, hue, and saturation for increasing the effective dimensionality of the display space [6].

Apart from the glyph based representation various other techniques like stream-tubes, stream-surfaces and hyper-streamlines have been used for tensor topology visualization. Vadim et al. [5] used the immersive environment for spatial exploration of NLC data.

2 MOTIVATION

Research in finding topological defects in the NLC data deals with the issues of exploring, filtering and efficient rendering. Effective visualization of NLC data requires the visualization of tensor, vector and scalar data in a composite view. High dimensionality of the data introduces a lot of challenges in the efficient visual encoding and realtime interaction [5]. Most of the existing techniques has focused on Diffusion Tensor MRI, stress and strain tensor data sets to visualize topologies or individual tensors. NLC visualization is a challenging problem due to the nature of data which comprises of the traceless tensors and vectors over the unstructured grid. Unavailability of any existing technique or tool for addressing the above requirements has been major motivational factor for our work.

2.1 Background and Data

Topological defects in the NLC are characterized by the sudden change of the orientation director vectors. Often this is caused by impurities in the liquid crystal that bond with the liquid crystal molecules, or an area of the liquid crystal that is in the liquid or solid state [3].

Data used for the visualization is computed by solving PDEs

*Department of Computer Science and Engineering, Bagley College of Engineering, Mississippi State University, MS 39762. E-mail: km223@erc.msstate.edu and tj@acm.org

†Department of Electrical and Computer Engineering, Bagley College of Engineering, Mississippi State University, MS 39792. E-mail: mall12@msstate.edu

over an unstructured grid. A solver generates a symmetric second-order tensor, vector and scalar values at each grid point for the collection of molecules in the associated volume. The grid size is of the order of 120K triangles. An application to visualize this data has been developed on a Linux platform using C++, OpenGL, KDevelop and the wxWindows toolkit.

3 DATA EXPLORATION TECHNIQUES

Each step in the visualization system helps the user in finding the relevant data and performing effective visualization of the NLC data.

3.1 Timeline View

Timeline visualization captures the critical information for each time step. To study the defects in the NLC, director orientation is a very critical parameter as it suggests possible defects in the structure. Each image of the timeline shows a scalar order (nS) distribution with histograms of the nS along each coordinate axis. This assists the user to correlate the nS distribution over the complete volume space or an individual dimension and identify the area where major change is occurring. Figure 2 illustrates the mapping of 3-D space to an 'oriented stick' and histogram diagram which is used to identify the relevant time steps.

Figure 2: Mapping of scalar order parameter from 3D to 2D space

3.2 Parallel Coordinate view

Subsequent to the timeline exploration, an identified timestep is loaded into the parallel coordinate view. This view shows the relationship between the nS and nS orientation vector (Figure 1). Data points are mapped to a linear gray color map based on the nS value of that point. Linear mapping is found to be more effective than the logarithmic scale, as it is easier to follow the gray lines. Gray color mapping helps in identifying the areas of sharp contrast, which suggests change in nS value around that location.

3.3 Glyph view

The user can select the relevant nS value range in the parallel coordinate view through brushing. It shows the associated tensor points in the glyph view window. All the basic 3D interaction techniques like scaling, zoom and trackball movement are provided for exploration. Filtering in the parallel coordinate view is intended to reduce the relevant data points for glyph view and thus reduce visual clutter and complexity. The 3-D view is useful in exploring the region of the data space where possible defect may occur and in getting detail information about the tensor and scalar parameters at that point as shown in the right image of the Figure 1. This image shows the ellipsoidal glyph at each grid point in the small crystal volume.

4 RESULTS

Preliminary results of our system shows that multi-level visualization is very effective in filtering data and focusing on exploration process. In a typical scenario, user loads the required time steps into the timeline view, that provides the information about the change of director orientation distribution over each timestep. On selecting the relevant timestep, parallel view shows the details of orientation vector. Subsequent selection of the nS value range in parallel coordinate loads the selected data points in the 3-D view for the detailed analysis. Interactive updating of any parameter will results in the updating of the views.

User input suggests that the current visual encoding is ineffective in conveying complete information as it ignores the grid structure. Also, while visualizing complete data space in 3-D introduces a lot of visual clutter.

5 CONCLUSION AND FUTURE WORK

In this abstract we presented the new NLC data exploration and visualization system for finding crystal defects. This system uses the timeline and parallel coordinates for increasing exploration efficiency and glyph based depiction for detailed view.

The described work is being enhanced to facilitate improved visualization using different approaches such as new interaction techniques and efficient visual encoding for director and automated disclination algorithm. Director value distribution needs to be density weighted in order to convey the unstructured grid information. Other automated filtering and distortion techniques are being explored for reducing visual-clutter of parallel coordinate visualization. Apart from interface enhancements, we are still exploring novel ways of visualizing tensor and vector data of unstructured grid in an interactive manner.

6 ACKNOWLEDGMENT

This work is sponsored by the National Science Foundation EP-SCoR program via award #0132618. We thank Dr. Rajendran Mohanraj of the SimCenter at the Engineering Research Center for providing the crystal simulation data and explaining the details about the nematic liquid crystals.

REFERENCES

- [1] G. L. Kindlmann. Superquadric tensor glyphs. In *VisSym*, pages 147–154, 2004.
- [2] D. H. Laidlaw, E. T. Ahrens, D. Kremers, M. J. Avalos, R. E. Jacobs, and C. Readhead. Visualizing diffusion tensor images of the mouse spinal cord. In D. Ebert, H. Hagen, and H. Rushmeier, editors, *IEEE Visualization '98*, pages 127–134, 1998.
- [3] N. Morrtram and C. Newton. Introduction to q-tensor theory. Website of Department of Mathematic, University of Strathclyde. <http://www.maths.strath.ac.uk/research/reports/2004/>.
- [4] F. H. Post, F. J. Post, T. V. Walsum, and D. Silver. Iconic techniques for feature visualization. In *VIS '95: Proceedings of the 6th conference on Visualization '95*, page 288, Washington, DC, USA, 1995.
- [5] V. Slavin, D. H. Laidlaw, S. Zhang, R. Pelcovits, G. Loriot, and A. Callan-Jones. Visualization of topological defects in nematic liquid crystals using streamtubes, streamsurfaces and ellipsoids. *IEEE Visualization 2004 Poster Compendium*, October 2004.
- [6] C. Ware. *Information Visualization: Perception for Design*. Morgan Kaufmann Publishers, second edition, 2004.
- [7] C. Westin, S. Peled, H. Gudbjartsson, R. Kikinis, and F. A. Jolesz. Geometrical diffusion measures for MRI from tensor basis analysis. In *ISMRM '97*, page 1742, Vancouver Canada, April 1997.