Nanoscale Visualization: Transfer Function Exploration

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August 7, 2003

Visualization plays an important role in the modern scientific process. In an era where the means of generating data through natural inquiry or simulation have vastly exceeded the power of direct analysis, tools to interpret and explore the data are crucial to the continued pursuit of knowledge. The field of visualization aims to bridge the gap between raw data and natural human perception through visual cues. One critical open problem in the field deals with how to create a meaningful transfer function. A transfer function is some parameter mapping between the data and its visual cues: opacity, color, or shading. The data represents a volume, where each point in the data is some measured value in three-dimensional space, such as density. The possibilities for a transfer function to describe any given dataset are endless.

In a visualization system with the transfer function parameters properly set, the salient points of a data set can be easily observed. Much research has been done to discover a more intuitive approach to volumetric parameter setting. He et al. have proposed interactive and automated systems based on genetic algorithms to *discover* "appropriate" transfer functions [1]. On the other hand, Bergman et al. have proposed a procedural system that is based on an intuitive front-end built atop a library of known colormaps [2]. Marks et al. move towards a system that tries to pick a statistically diverse subset of renders from the entire render set [3]. These renders are then relationally mapped for the end-user to explore. All these techniques attempt to abstract visualization parameters from complex input vectors into systems that allow any user to freely explore the render-space of a given data set. This aids in the discovery and highlighting of important data features without the need for someone who is a visualization expert.

A natural progression from the easing of parameter setting is the introduction of additional information to visualize. This additional information can be in the form of higher dimensional data sets or multi-volume datasets. There are many methods currently being researched that elucidate artistic techniques and apply them to volumetric data [4, 5]. These *volume illustration* methods allow for the synthesis of multiple sets of data into one view-plane by abstracting the data beyond a simple shape representation. Wilson et al. address the issue of applying these volume illustration techniques to two distinct volumes [6]. They also offer solutions for other problems with viewing multiple volumes, such as: hardware limitations and techniques for visualizing the fusion of volumes.

The research in this presentation focused on transfer function design and how it can provide nanotechnology researchers with new ways to *explore* their data and gain a deeper understanding of what the data represents. Three sub-fields of nanotechnology were analyzed to see how visualization techniques for this data could be implemented or improved: theoretical nanoscale device simulation, experimental structural cell biology, and theoretical molecular modeling, to see how visualization techniques for this data could be implemented or improved. The initial work dealt with the basics of viewing this data. Each dataset was represented in a slightly different format and had to be converted into a common usable format. Next, the aforementioned transfer function and feature enhancement techniques were analyzed for their application to the datasets. Some methods provided a software implementation which could be applied directly to the data. Other methods needed to be analyzed based on the results provided in the literature. The volume renderer, Simian [7], was eventually chosen as a base package to work from. Simian is a solid, feature-rich, hardware accelerated volume renderer based on the idea of multi-dimensional transfer functions [8]. It also includes a number of widgets to interact with the data such as: dual-domain interaction, a data probe, and clipping planes.

Once all three datasets were viewable from Simian the research focus turned toward the device modeling data. The goal was to explore the local density of state in nanoscale MOSFETs and discover features such as tunneling, as well as the ability to interactively view the effect that changing gate biases has on the local density of state. Simian was extended to allow for the visualization of multiple discrete bias points in a time-variant manner. Since three-dimensional bias-variant data was not available, a large part of the research was directed at using the nanoMOS [9] simulator itself. The simulator can run in parallel on a clustered supercomputer. After some basic analysis of the nanoMOS code, the simulator was run for discrete voltage bias points, so the results could be used with the modified version of Simian and simulate real-time gate-bias interaction. Unfortunately, the initial batch of simulations returned incorrect data. Thus, visual results of pseudo-real-time interaction with the gate-bias points are pending a corrected version of the nanoMOS code.

In general, this research resulted in the compilation of some initial tools and techniques to aid in nanoscale data exploration. Further work must be done in the application and synthesis of more advanced visualization techniques towards nanoscale data. After new nanoMOS data is harvested it will be interesting to characterize when features such as tunneling occur and highlight them visually.

References

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