

Scientific Visualization of Superconducting Materials

The research objective is to begin development of a real-time visualization tool for superconducting materials. This project involved participation from the Visualization Task Group and the Computational Materials Sciences group. This tool will be used to communicate the structure and properties of superconducting materials. Simulations of superconducting materials are an important scientific application area which utilizes ORNL's supercomputers. The tool will be written using calls to the OpenGL graphics library. By programming the tool with OpenGL calls, it will be useful with a variety of output devices ranging from desktop computers to tiled displays. This tool also has several important advantages which were indicated by my mentors. These advantages included reading custom data formats, changing data visualization representations desired by the researchers, and providing interactivity with the visualization such as zooming in and focusing on different levels of detail in the material structure. Interactivity will allow researchers to use the tool to emphasize or deemphasize points during a presentation. Tiled displays used by the Visualization Task Group include the 6-panel LCD array and the massive 27-panel EVEREST visualization environment. The Chromium software which distributes geometry generated by OpenGL programs and puts the right parts of the visualized geometry on the correct panels of the projection array was used on a Linux workstation to compile and build about 2 dozen OpenGL study programs downloaded from Neon/Helium Productions (<http://nehe.gamedev.net/>). Celestica was used to understand the possibilities of programming in OpenGL. An investigation of VMD, a production visualization package for molecular dynamics, provided an understanding of its high-end capabilities. Based on an understanding of OpenGL, an interactive program for moving a molecule around on an undulating surface was developed. This program will be the basis for more complicated real-time programs used in visualizing and investigating superconducting materials datasets.

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