

Scientific Visualization of Superconducting Materials

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<http://www.csm.ornl.gov/Internships/abstracts/JermaineWalker.pdf>

Abstract

My objective is to begin development of a real-time tool for visualizing superconducting materials. This tool will be used to communicate the structure and properties of superconducting materials and will be written using calls to the OpenGL graphics library, making it useful with a variety of output devices ranging from desktop computers to tiled displays. The advantages of this tool include 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.

Methods

OpenGL Functionality Visualization Tool Functionality

- | | |
|--------------------------|------------------------------------|
| 1. 3D shape/adding color | 1. Atom/element representations |
| 2. Blending/rotation | 2. Rotation |
| 3. Sphere mapping | 3. Z scaling (zoom in/out) |
| 4. Flag effect | 4. Parameter mapping onto surfaces |
| 5. CG vertex shader | |

Software Tools

1. AVS
2. VTK
3. VMD
4. vi
5. OpenGL libraries
6. Chromium

Rendering for Materials Science

1. 3D image
2. 2D plane
3. Unit cells
4. Atoms/elements
5. Electron flow

Hardware Tools

1. Linux workstations
2. LCD array
3. EVEREST environments
4. Render clusters

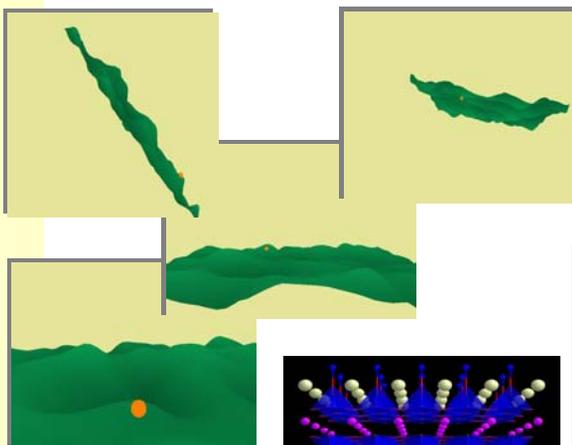


Figure 1. Interaction of materials sciences

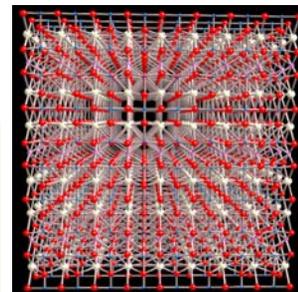


Figure 3. 3D Crystal model

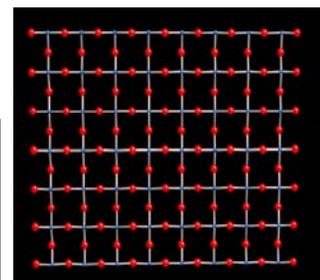


Figure 4. 2D Sliced crystal

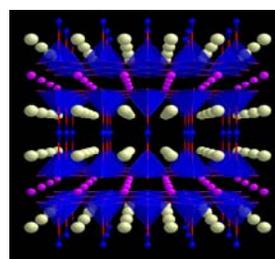


Figure 2. 3D Crystal model

Conclusion

To complete my study of existing tools, I investigated VMD, a production visualization package for molecular dynamics, to understand its capabilities. Based on my understanding of OpenGL to date, I have written an interactive program for moving a molecule around on an undulating surface. This interactivity is important for understanding the characteristics of electron flow in the superconducting lattice as well as the properties of the Hubbard model utilized by the materials scientists also involved in this activity. The program will be the basis for more complicated real-time programs used in visualizing and investigating superconducting materials datasets.

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