LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

Optimizing Stereographic Visualization of Atomistic Configurations

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Abstract

- Current research focuses on the Cave Automatic Virtual Environment (CAVE) to visualize simulation results.
- C/C++ Visual Studio project from a previous LA-SIGMA REU [1] is modified to improve the display and optimized to interactively handle a larger number of atoms.
- For test purposes a periodic body centered cubic (BCC) lattice is visualized on a desktop and the CPU time to display one frame measured as an average over 100 frames.
- Results should apply to configurations with moving atoms also.

The CAVE

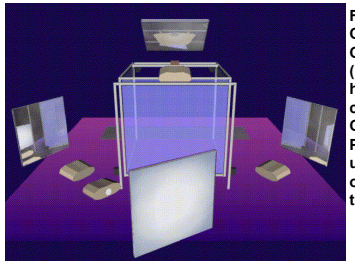

Fig 1. Schematic of the CAVE at Southern's College of Engineering. (Figure from http.cs.uic.edu/~kenyon/conference/GILKY/CAVE_DOD.html) Projection is via mirrors used to set the correct optical distance equal to the projector's throw.

- The CAVE at Southern's College of Engineering (CoE) (Fig. 1) is where this work, on stereographic visualization of molecular configurations, will be used.
- The CAVE is an 8 ft x 8 ft x 8 ft space with 4 displays (3 displays on screen-walls and 1 display on the floor).
- Active stereo with eye ware synchronized to separate left & right eye images displayed in rapid sequence allow the user to see in stereo.

1. G.R. Wrigth, S. Kodiyalam, A. Jana, "Stereographic Visualization of Molecular Configurations in a CAVE" LA-SiGMA 2011 REU Report.

Methodology

- CAVE-Library based C/C++ project has separate threads for the main and display loops.
- Main thread currently generates a fixed BCC lattice but is otherwise an empty loop that may be used for reading in simulation results.
- Display loop begins with a one-time call to a function initializing the display by setting directional lighting with ambient, diffuse, and specular qualities.
- Navigation function within the display loop enables translation, rotation, and scaling of the entire scene.
- Display function applies the navigation transformation and calls a "Make Display List" function.
- Make Display List function uses the atomic position and atomic type arrays and creates the display of atoms of two types and bonds between them using OpenGL functions and either (1) Calls to sphere creating [1] and cylinder creating functions using the GLU library, or (2) Calls to display lists creating the objects with additional OpenGL calls as needed.

Results: Display improvement

- Display of bonds improved by the use of cylinders instead of lines (Fig. 2)

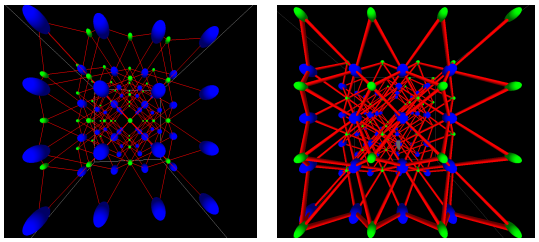

Fig 2. Improving the display of bonds. (Left) shows the display of bonds as lines as before [1]. Right shows the display of bonds as cylinders. Cylinders are created out of primitives corresponding to 20 slices (along the circumference) and one stack (along the length).

Results: Faster code execution

- Code execution faster when using display lists (Figs. 3, 4, & 5).

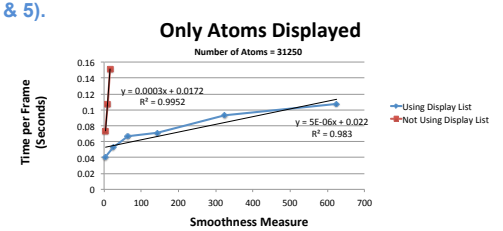

Fig 3. Execution time for the display of atoms varies linearly with the atoms' display smoothness measure as before [1]. Using display lists for the atoms increases the execution speed by more than an order of magnitude. The curve without display lists has only one data point for illustrative purposes.

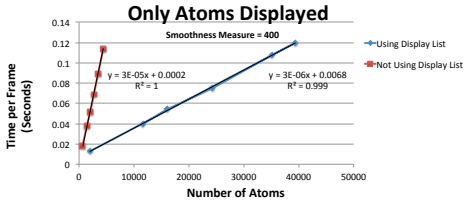

Fig 4. Execution time for the display of atoms varies linearly with the number of atoms as before [1]. Using display lists for the atoms increases the execution speed by roughly an order of magnitude.

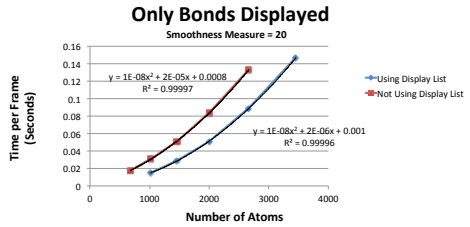

Fig 5. Execution time for the display of bonds varies quadratically with the number of atoms as before[1]. Using display lists increases the execution speed. However the quadratic dependence limits the number of atoms that can be handled interactively to much smaller values as compared to when only atoms are displayed (Fig. 4).

Conclusion and Future Work

- Display lists increase the number of atoms and bonds that can be visualized interactively.
- Current limitation on the display of bonds may be overcome by the use of linked lists.

Acknowledgements

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