OPTIMIZING STEREOGRAPHIC VISUALIZATION OF ATOMISTIC CONFIGURATIONS

Cole Vanderlick[1], Sanjay Kodiyalam[2], Amitava Jana[2]
[1]REU Student; Petroleum Engineering, Louisiana State University, Baton Rouge, LA 70803
[2]Mechanical Engineering, Southern University and A&M College, Baton Rouge, LA 70813

Outline

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Motivation

- **Interactively visualize large scale atomistic configurations to discover mechanisms for the simulated phenomena**

Objectives

- Improve the display of bonds from lines to cylinders
- Make the code run more efficiently to be able to handle larger number of atoms
- Identify future tasks to improve the efficiency of the code
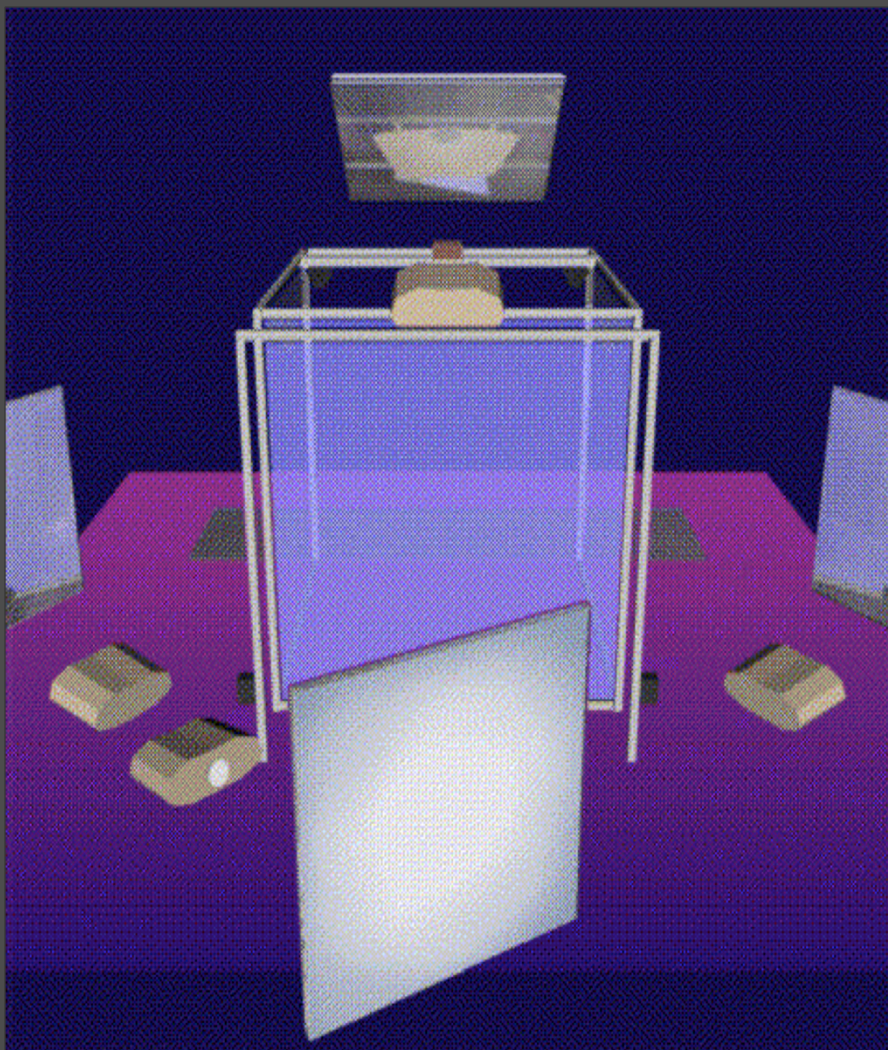
The CAVE

- Cave Automatic Virtual Environment (CAVE)
- 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.
- This CAVE is where this work, on stereographic visualization of molecular configurations, will be used.

Methodology

- CAVE-Library based C/C++ program 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

Methodology

- **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 and cylinder creating functions, or (2) Calls to display lists creating the objects with additional calls as needed**

Results: Display Improvement
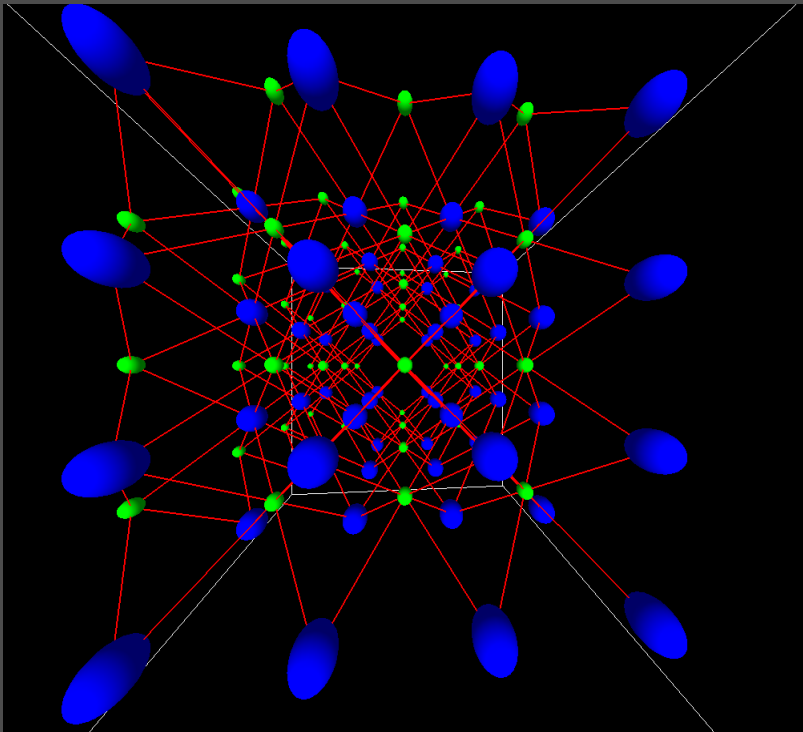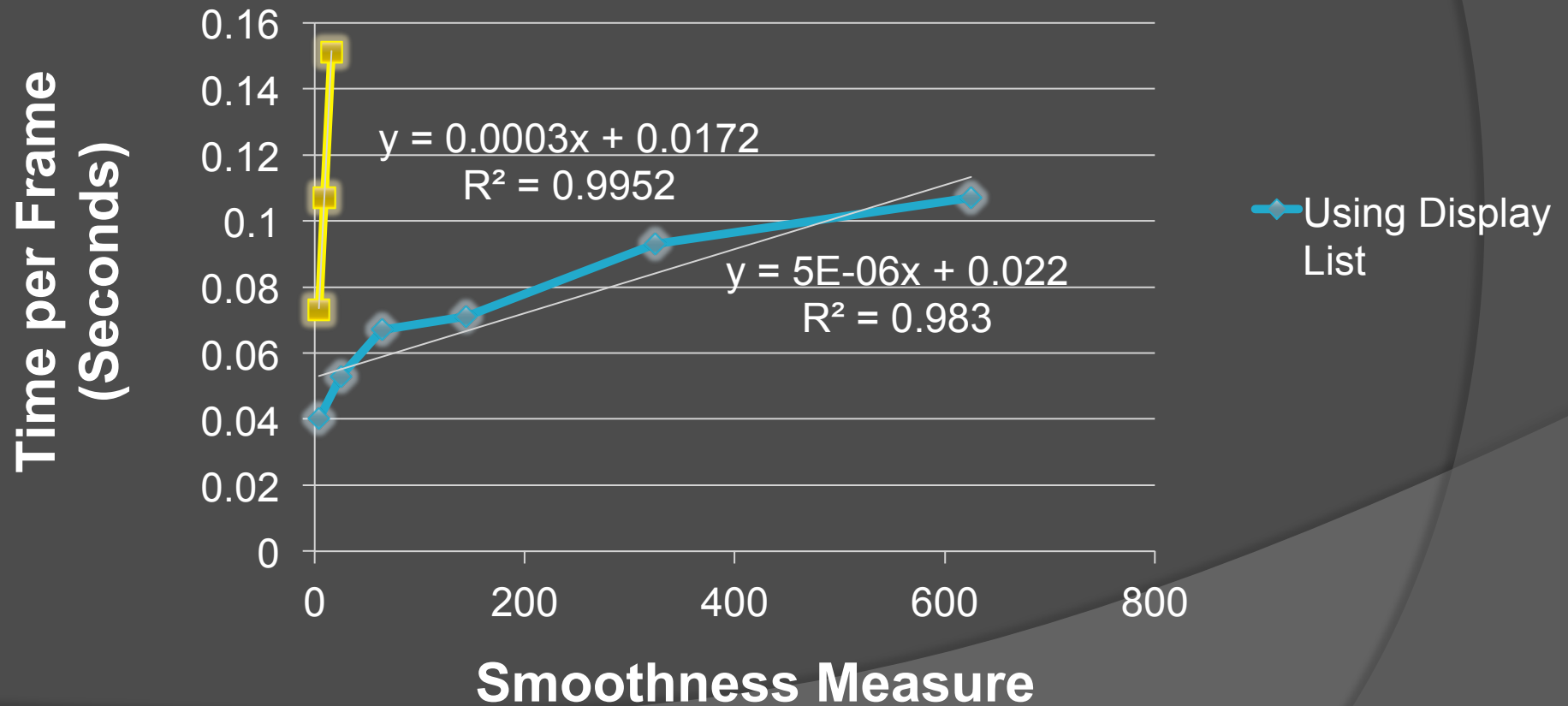

o **Shows the display of bonds as lines**
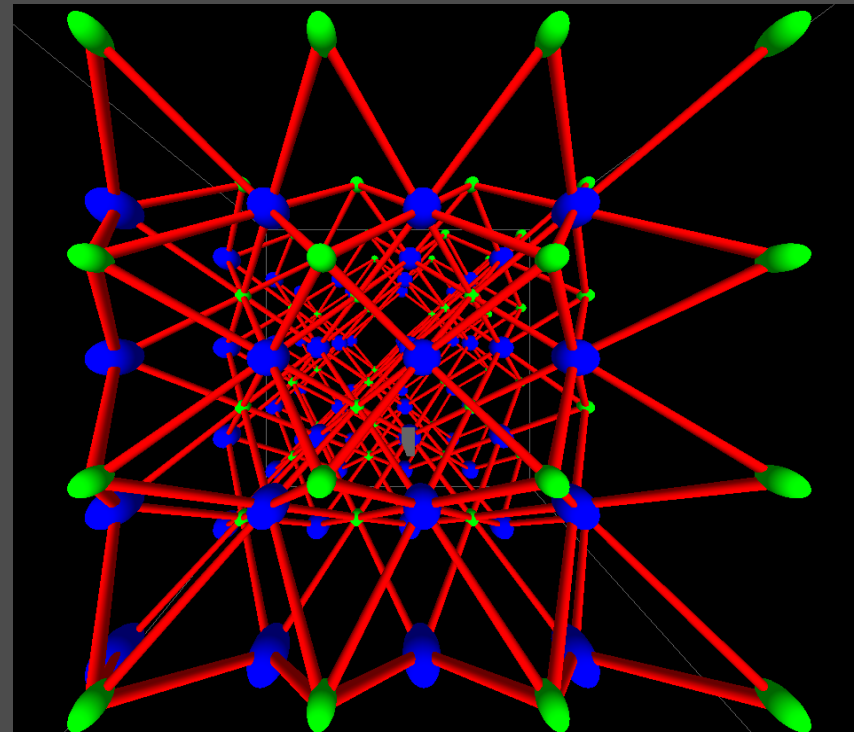
o **Shows the display of bonds as cylinders**
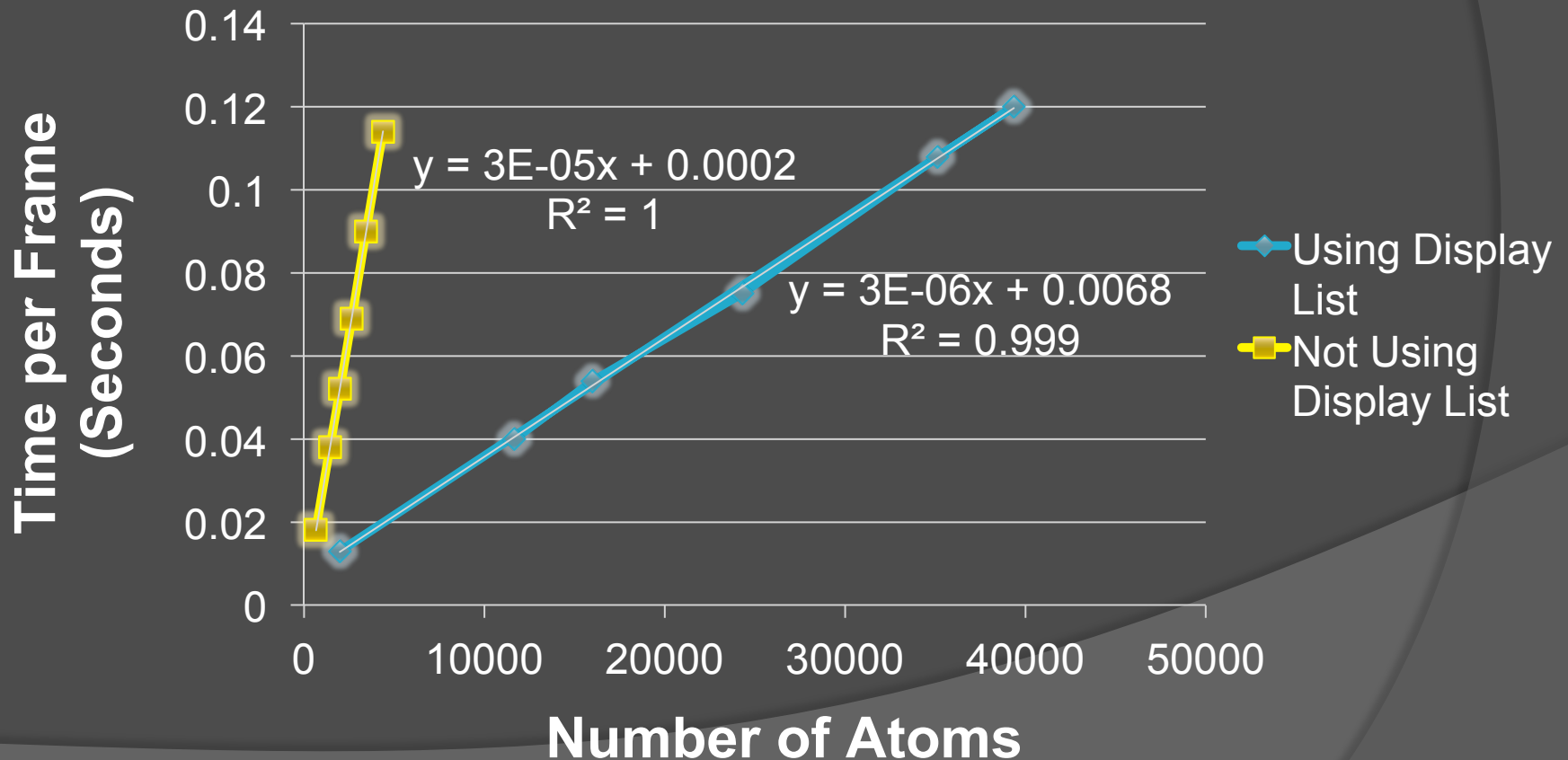
Results: Faster Code Execution

Only Atoms Displayed

Number of Atoms = 31250

$y = 0.0003x + 0.0172$
$R^2 = 0.9952$

$y = 5E\text{-}06x + 0.022$
$R^2 = 0.983$

Using Display List

Time per Frame (Seconds)

Smoothness Measure

Results: Faster Code Execution

Only Atoms Displayed

Smoothness Measure = 400

$y = 3E{-}05x + 0.0002$
$R^2 = 1$

$y = 3E{-}06x + 0.0068$
$R^2 = 0.999$

Time per Frame (Seconds)

Number of Atoms

Using Display List

Not Using Display List

Results: Faster Code Execution

Only Bonds Displayed

Smoothness Measure = 20

$y = 1E-08x^2 + 2E-05x + 0.0008$
$R^2 = 1$

$y = 1E-08x^2 + 2E-06x + 0.001$
$R^2 = 1$

Time per Frame (Seconds)

Number of Atoms
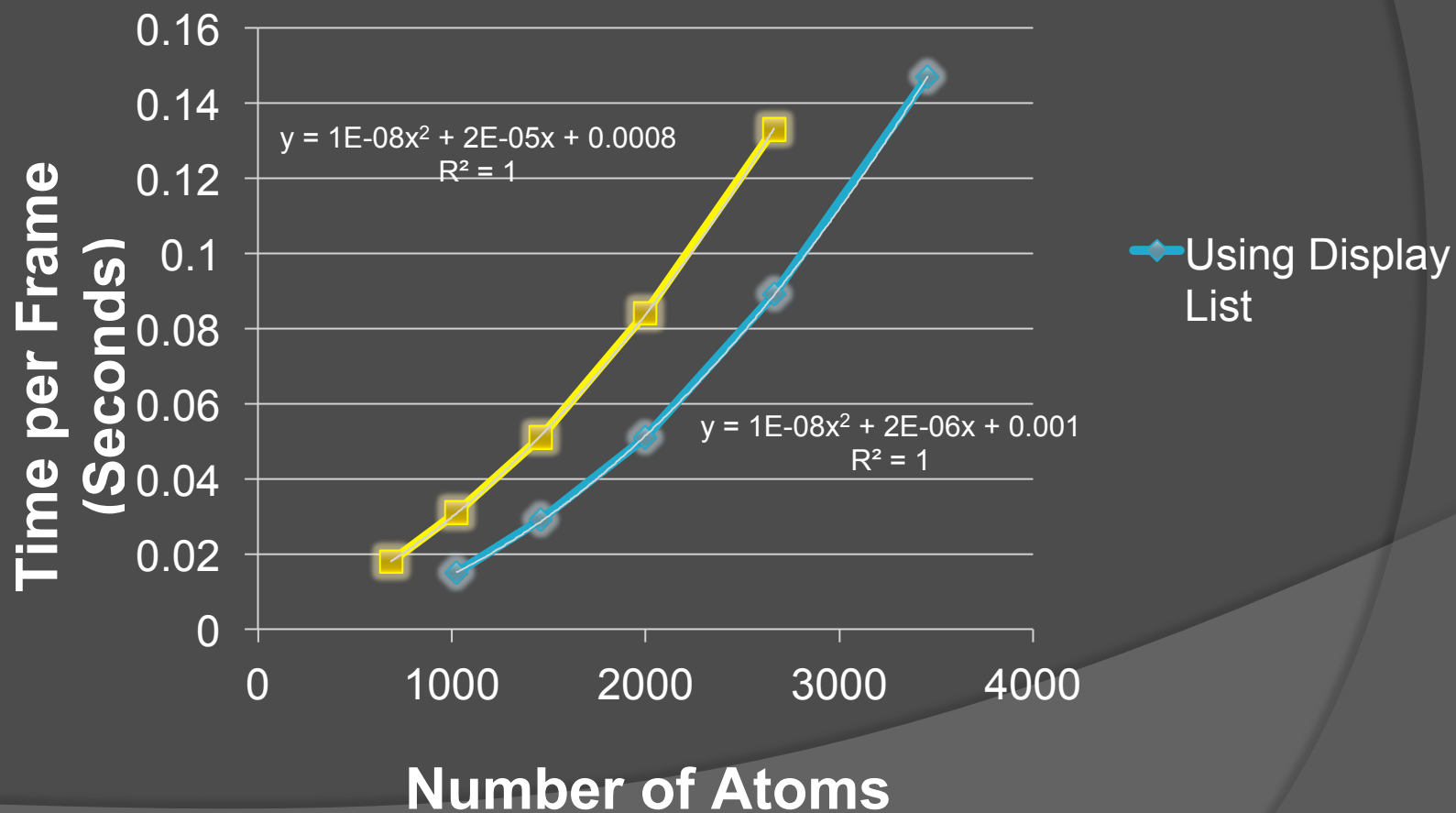
Using Display List

Conclusion

- **Display lists increase the number of atoms and bonds that can be visualized interactively**
- **Bonds, connected by lines, have been converted to cylinders to give a more realistic view**
- **Future Work: Current limitation on the display of bonds may be overcome by the use of linked lists**

Acknowledgements

QUESTIONS?!?!