Stereographic Visualization of Molecular Configurations in a CAVE

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Introduction:

•Current research in computational sciences focuses on virtual reality systems with emphasis on the Cave Automatic Virtual Environment (CAVE) for the visual inspection of the computed results.

•We have therefore begun the construction of such a visualization-analysis program with the eventual goal of being able to visualize ~million-atom configurations.

•A Visual Studio C/C++ project for the visualization of atoms and bonds in a molecular dynamics configuration is developed and its performance (CPU time taken versus number of atoms) is determined.

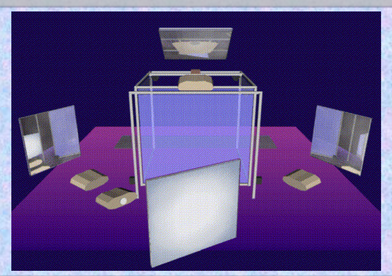


Figure 1. Schematic of the CAVE

The Cave:

This work, on visualizing atomistic configurations, was conducted at the CAVE at Southern's College of Engineering (CoE) (Fig. 1).

•This CAVE is an 8 ft x 8 ft x 8 ft space with 4 displays (3 on screen-walls and one on the floor).
•Images projected via mirrors setting the optical distance = the projector's throw
•Active stereo: Separate left & right eye images synchronized with eye-ware
•Position and orientation of two sensors (eye-ware and joystick) tracked
•CAVE driven by 2-node cluster: Master (collects sensor info) & Display (drives projectors)
•Perspective transformations required for displays automatically carried out by CAVE-library using eye-ware sensor information
•Joystick sensor information accessible to the visualization application for use in updating the display.

References:

[1] Figure from http.cs.uic.edu/~kenyon/conference/GILKY/CAVE_DOD.html

[2] D. Driggs, S. Kodiyalam, K., A. Jana, "Modeling Virtual Cooperative Robots," Proceedings of the 2011 ASEE-GSW Conference, March 2011, Houston, TX., Session FC1-1.

Methodology

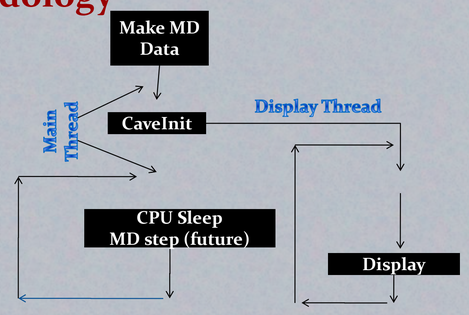
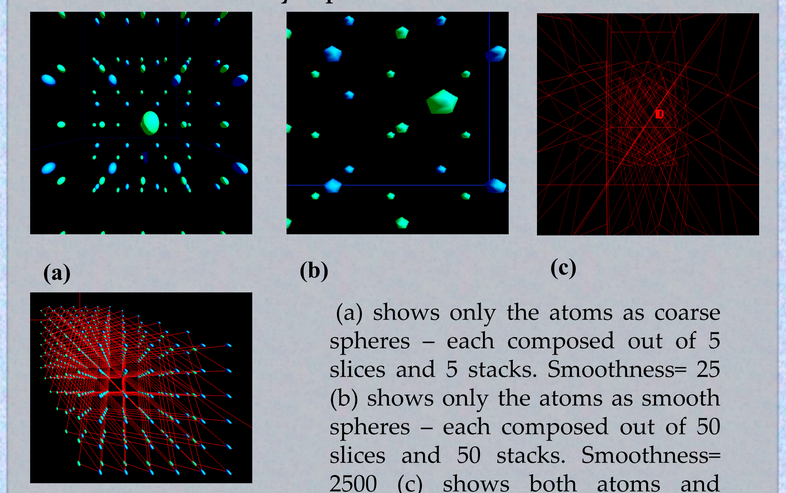


Figure 2: Flow Chart of Cave Init

Four threads were utilized to generate the complete code.
•Main Function-Creates an array corresponding to Atomtype(integer), position & velocity(3 double precision numbers)
•InitializationDisplayFunction- Sets Ambient, Diffuse, and Specular lighting using OpenGL
•Navigation-Adopted from earlier work[2]. This Enables the translation, rotation, and scaling of entire virtual world
•Display Function-The atoms are displayed in a loop. The atom's positions are set using glTranslate before the call to gluSphere. GluSphere creates the sphere. The smoothness of the spheres are determined by the number of slices(longitudes) and stacks(latitudes).
•GlPushMatrix-glPopMatrix is set over each display.
•The Bonds are displayed in a double loop. Only "nearest neighbor" atoms are bonded. OpenGL Draw_Lines function is then implemented.
The colors are set by OpenGl colors and material.



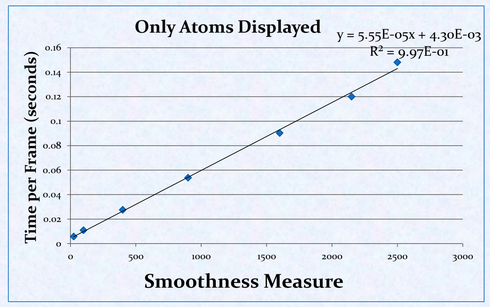
(a) **(b)** **(c)** **(d)**

(a) shows only the atoms as coarse spheres – each composed out of 5 slices and 5 stacks. Smoothness= 25 (b) shows only the atoms as smooth spheres – each composed out of 50 slices and 50 stacks. Smoothness= 2500 (c) shows both atoms and bonds. (d) shows only the bonds.

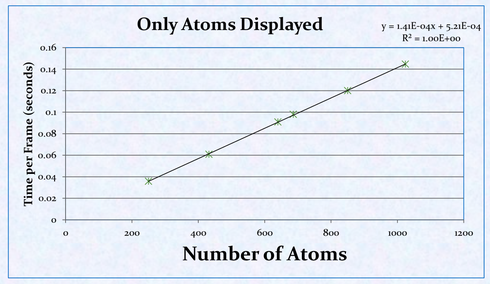
Results

The CPU-timing is carried out on the development platform: a desktop with a non-stereo "CAVE Simulator" display.

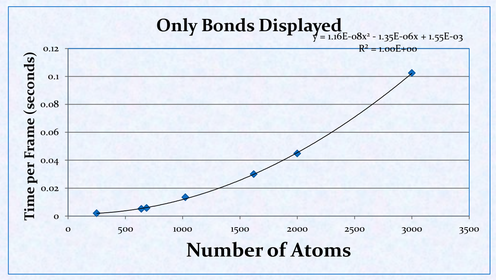
Results



•Constant Number of Atoms (1024)
•This graph shows the time required for displaying one frame of atoms only at different smoothness measures.



•Constant Smoothness Measure(2500)
•This graph shows atoms increasing as time increases.



•This graph shows bonds only as a quadratic function (Number of atoms^2).

Conclusions

•CPU time required for display of atoms alone scales linearly with the total number of atoms / OpenGL primitives
•The display of bonds alone is quadratic in the total number of atoms.
•The performance of the current version of the project leads to an upper bound in the number of atoms that can be handled, with an interactive frame rate of 10 frames per second, of 706 and 2913 respectively for the display of atoms or bonds alone.

Future Work

•To increase atoms' display speed by having a variable smoothness measure for the sphere-atom depending on the perspective angular width of the atom.
•Bond display can be made to scale linearly with the number of atoms by using linked and neighbor lists.
•A more robust display of the bond using cylinders can be attempted.

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