Visualization of Molecular Structure by Emphasizing Conformational Changes

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Abstract

Three-dimensional visualizations of molecular structure can aid scientists from different disciplines in communicating their ideas more efficiently. Current visualization techniques fail to illustrate uncertain factors like conformational changes and hydrogen bonding migration. Efforts have been made to create three-dimensional molecular visualizations with emphasis of the conformational changes. The resulting images were evaluated by an informal user study.

Methods

Before implementing any visualization techniques, many potentially useful methods were evaluated with the help of existing molecular visualization and image editing tools. The images from these preliminary studies were assessed to find suitable techniques that could be implemented within the given time frame.

The techniques chosen from the preliminary study were implemented thereafter. The visualization techniques applied include different representations for molecular structure, varying degrees of color, shade and transparency for different conformations, and realistic shading effects. The program was built by cutomizing VMD, a well known open-source molecular visualization software. Efforts have also been made to make the program as easy to use as possible for novice users.

Both preliminary and final images generated were subject to informal user evaluations. The test subjects were chemistry graduate students, with considerable experience in using various molecular visualization tools.

Results

New techniques for rendering molecular structure with the emphasis of uncertain conformational factors have been developed.

We rendered images combining various representation methods for different molecular conformations. Various strategies were used to represent simple and complex molecules. The sample image shown in figure 1 is a visualization of a simple molecule with three conformations and the image in figure 2 shows a visualization of a complex molecule. The program generates an interactive visualization of the molecule. To generate a more realistic image the program can also output the visualization to a file readable by a ray tracer (POV-Ray). The resulting publication quality ray traced image shows more realistic effects such as transparency and shadows.

User studies were conducted with a large number of images generated by the program. The results showed that the test subjects thought it was relatively easy to identify the conformations and their relative ratios in renderings with less than four conformations. Techniques such as the use of shadows were found to be helpful in visualizing simple molecules, but were ineffective for more complex ones (greater than 200 atoms). Also, users had difficulty with depth perception in complex molecules when transparency was used to represent the static portion of the molecule.

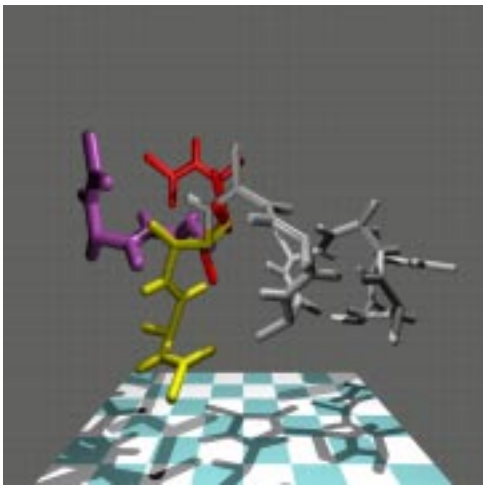

Figure 1. Visualization of Alanin showing three possible conformations in yellow, purple and red. The static portion of the molecule is shown in gray.

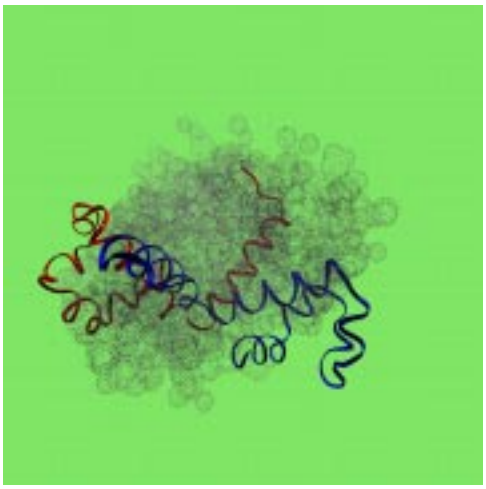

Figure 2. A complex molecule with two conformations. The dotted spheres in the background represent the static portion of the molecule.

Conclusions

We have succeeded in generating publication quality images of conformation changes in molecules. Having a single image representation of conformational changes not only saves space in publications, but also provides the viewer with a better understanding of the relative probability of each conformation. The user studies provided us with valuable information on choosing visualization strategies for molecules with vastly different sizes, shapes and compositions.