



BCB/MGET Thesis Seminar

CAVEMol: an immersive 3D molecule viewer

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Abstract:

As the number of solved molecular structures deposited with the Protein Data Bank (PDB) increases, so too does the desire for more advanced ways of using this data. Traditional applications for viewing and manipulating molecular structures create a computer-generated model on a standard desktop computer screen. The display may employ some method of stereography to create the illusion of depth, but generally the user just sees a flat image. The user is able to interact with the molecule by magnifying it to get closer look at a particular area of interest, or by rotating it along an arbitrary axis, thus allowing all sides of the molecule to be seen, though only one side is in view at any given time. The user may also be able to see changes in the molecule over time whereby each conformation of the molecule is a separate frame of an animation, or they may even be able to make modifications to the structure in real time. Regardless of the amount of control the user has over the molecule, however, one thing remains the same: the user experiences the molecule as though it were an object floating behind the monitor screen which they can indirectly control using a mouse or other pointing device.

An immersive environment, on the other hand, provides a new paradigm for molecular visualization, allowing the user a much more realistic interaction with the molecule. The user becomes part of the viewing experience, traversing a molecule as though walking or flying within it. The molecule can completely surround them on all sides, giving them a true sense of the size and shape of the molecule in three dimensions. The user may also interact with the object directly, moving and rotating it with their hands rather than a mouse.

This approach should prove particularly valuable for operations such as “interactive docking,” which allows a user to manipulate the interface between two molecules to identify favorable interaction sites. While this can be done to a degree in today’s desktop molecule viewers, the operation is difficult and time consuming. Because today’s viewers are limited to a flat screen display, a user can only attempt to dock two molecules in two dimensions at a time. When the structure is rotated, more often than not the third dimension is not properly aligned. Realigning the third dimension invariably breaks one or both of the first two. The result is a long and frustrating cycle of alignment rotation and realignment. By allowing direct manipulation in all three dimensions simultaneously, the immersive perspective eliminates this cycle.

This thesis presents the design and implementation of CAVEMol, a molecular visualization application for immersive environments. I will also give an overview of molecular visualization and immersive environments, and then discuss future work that can be done in this area as well as applications where molecular visualization in an immersive environment can be particularly valuable.