Accurate 3D Modeling of User Inputted Molecules

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Abstract

In order to better understand the structure of molecules, chemists create 3 dimensional molecular models. These models help explain reactivity, polarity and many other characteristics pertinent to chemistry. In a large introductory chemistry class, it is too costly to provide each student with a physical modeling set. Software available online can also be costly. The goal of my research project is to create a free application that will allow users to generate 3D models of simple molecules through an easy and intuitive interface. Then, after the model is created, the application will position the atoms in the molecule correctly by using a Nelder Mead algorithm. My project will help users better understand the geometry of different molecules.

Background

In order to allow users to learn about the geometries of different molecules, my application will attempt to position the atoms correctly when the user chooses the "Auto-Position Atoms" option from the menu. This function will use a Nelder Mead algorithm to minimize the energy of the model. The Nelder Mead algorithm was created by Nelder and Mead in 1965, and uses the concept of a simplex in order to minimize a function in a many-dimensional space. (Price) A simplex is a polytope of N+1 vertices, with each vertex containing N dimensions; therefore, for a problem with two variables, the simplex is a triangle in 2D space, and for a problem with three variables, the simplex is a tetrahedron in 3D space. (See Figure 2) The algorithm begins with an original simplex, which must be large enough to avoid a local search that would end when a local minimum is found instead of the absolute minimum. The simplex should also not be too large because a large simplex could affect efficiency. (Kelly) The algorithm runs until it reaches a defined tolerance. My application uses a variation of the Nelder Mead algorithm outlined in "Convergence Properties of the Nelder--Mead Simplex Method in Low Dimensions," which contains five steps for each iteration of the algorithm: order, reflection, expansion, contraction and shrink. (Lagarias) Through these steps, the algorithm finds the minimum energy.

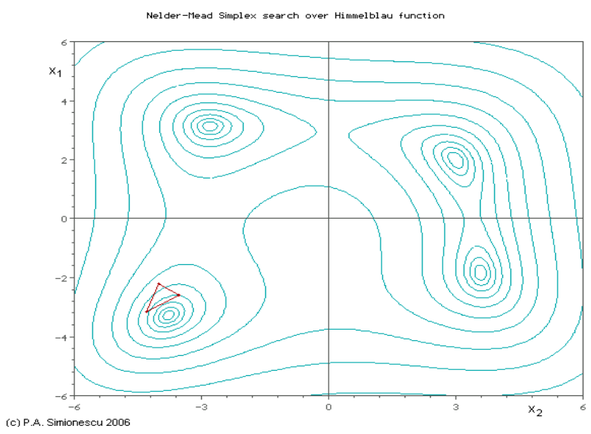


Figure 1: An example of the Nelder Mead algorithm using a simplex (red triangle) to find the minimum of a problem with two dimensions. (Image from web.cecs.pdx.edu)

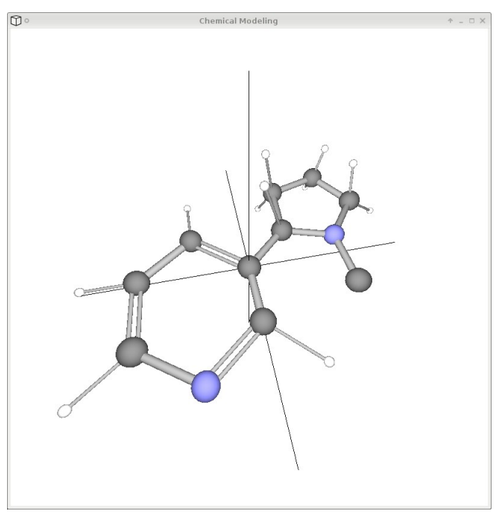


Figure 2: Model of nicotine created by using my application.

Development

In order to create a user friendly interface, I utilized OpenGL's ability to handle both the graphics and the user inputs. Models are created with atoms represented by spheres and bonds represented by cylinders. My application uses empirical values of atomic radii derived by J.C. Slater in order to draw atoms that are proportionally correct. (Slater)

I used a Neder Mead algorithm in order to have the my application orient the atoms of the molecules accurately for the user. The dimension (N) of the problem equals 3 * (the number of atoms) because each atom has a three values (x, y, z) . The Nelder Mead algorithm uses a simplex with N + 1 vertices in order to find the minimum of the energy function. Each vertex of the simplex represents an orientation of the current molecule.

The energy function that the Nelder Mead minimizes can be broken up into three parts. The first part tries to maximize the distance between each pair of non-bonded atoms. The next part of the energy function tries to get the distance between bonded atoms as close as possible to the actual values. These actual values are contained in a text file and were derived derived from experiments. ("Bond Lengths and Energies") The third part of the function tries to maximize all bond angles in the model. Since the Nelder Mead function tries to minimize the energy of the system, the minimum energy will occur when non-bonded atoms are as far apart as possible (real atoms do push away from each other), and bonded atoms are the specified distance apart.

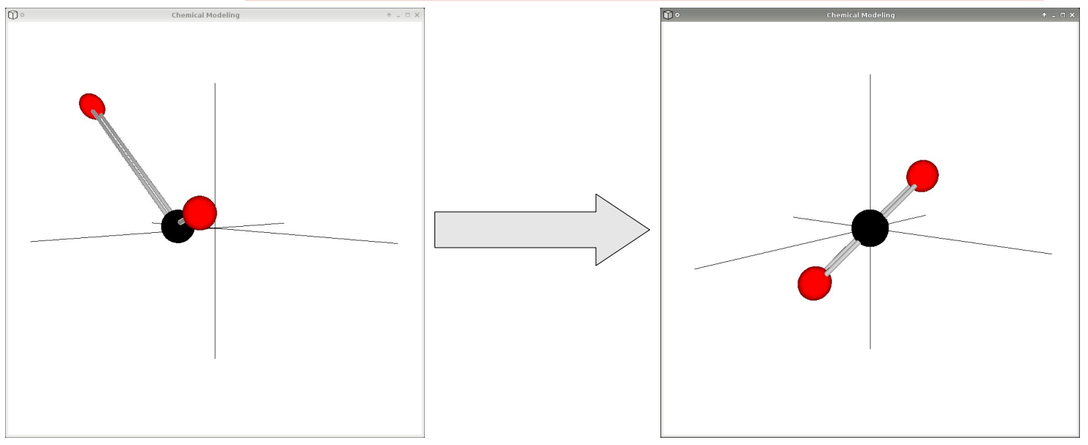
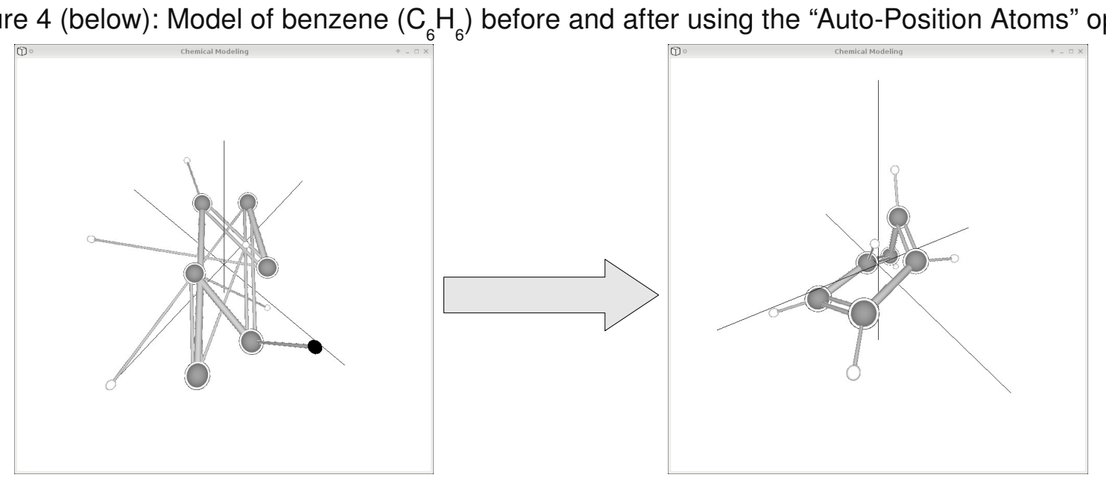


Figure 3 (above): Model of CO_2 before and after using the “Auto-Position Atoms” option.

Figure 4 (below): Model of benzene (C_6H_6) before and after using the “Auto-Position Atoms” option.



Results

The first part of my goal was completely met; all graphics and user interface components were tested and work as expected. The second goal of my project was not completely reached. First, polarity of atoms is not accounted for, so water will be drawn incorrectly. Second, the Nelder Mead algorithm does not work perfectly for every simple molecule. Specifically, as the number of atoms in the model increase, the error with the model created by the "Auto-Position Atoms" option increases. Molecules with only two atoms have no error; molecules with three atoms average a percent error less than .25%; the ring of carbon is created for a benzene molecule, which has 12 atoms (See Figure 4). Even though there are two problems with the Nelder Mead algorithm, the application would still be helpful for introductory chemistry students because it could, at the very least, provide a rough model of the molecule. However, fixing the two problems would allow the application to create more accurate models.