Computer Systems Lab 2007-2008: Research Paper Accurate 3D-Modeling of User Inputted Molecules

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Abstract

In order to better understand chemistry, chemists create 3D models of molecules. In a large introductory chemistry class, physical models are not viable because the supplies needed to give each student the opportunity to create even simple molecules are too costly. The goal of my research project is to create a program that would generate accurate 3D models of simple molecules, avoiding the cost problem with physical models. Therefore, since it is hard to find a modeling program that is free, my project could help students in introductory chemistry courses better understand the different shapes of molecules.

1 Introduction

The goal of my project is to create a free and simple program that will allow users, such as introductory chemistry students, to create models of molecules. These models will be rotatable and zoomable, allowing for a better understanding of the molecular geometry.

The first step to my project was creating the graphics for my models. The graphics for my project are a much simplified version of real molecules: spheres represent atoms and cylinders represent bonds. Nevertheless, the results are sufficient.

The second step of my project is creating the algorithm that will correctly orient the atoms in the molecule. Since there are many variables accounting for the actual orientation of the atoms and because I only have a limited amount of time, I will need to limit the number of accounted variables. With my set number of accounted variables, I will use an A.I. algorithm (hill-climbing) to correctly orient the atoms in the molecule. The first variable that I will account for will be the polarity of the bond. Once I get that working, I will continue to add more variables, creating a better model.

2 Background

A lot of research has been done on modeling molecules and the techniques to do so now have become quite advanced. Pharmaceutical companies have invested thousands of dollars in programs to predict orientations of new complex molecules. Large databases have been created, storing the orientations of thousands of molecules. Chemists have modeled everything from RNA to inorganic crystals. These programs have become increasingly more accurate over the years. However, the cost of these programs has also increased, and now very few people have access to them. Therefore, even today, a free program to model simple molecules would be helpful.

3 Preliminary Testing

Testing the graphic part of my program was simple; all I had to do was run it and see if my program created the intended model.

Now that I have most of the graphics done for my project, I will now be able to start working on my algorithm to correctly orient the atoms in the molecule. I will first start by only taking one variable into account: the polarity of the bond. Once I get that working, I will then add another. Once that one is working, I will start on another. Through this process, my program will start to produce accurate representations of different molecules.

In order to see if my program is constructing accurate models, I will compare my models with the actual/accepted models. By doing this, I will also be able to do error analyses. In order to thoroughly test my program, I will test many different molecules and compare my results with the actual orientations.

Dynamic testing will not work for my project because an atom can not bond with any random atom. Therefore, I will mostly use specific structural and functional testing and path and branch testing.

4 Results

My project currently allows users to create molecules by editing a few lines in the source code. A user can also rotate the model and zoom it in and out. These functions help users get a better picture of the molecule. However, many more functions, such as the ability to correctly orient the atoms, need to be implemented.