**20% Time Report**

**Purpose / Project Proposal:**

Our project attempts to mathematically model the electrical interactions of amino acids to predict their tertiary protein structures. The project will not attempt to model protein folding via the typical probabilistic guess-and-check approach. The goal, therefore, is to efficiently and accurately model the biological process of protein folding. As students, we hope to both learn about the biology behind the phenomenon and gain experience in computational scientific modeling. The idea for this project came when one of our members wanted to improve the standing guess-and-check model used to predict protein structures.

**Current Participants:**

Currently (and for the foreseeable future) Tyler Giallanza, Ian Johnson, and Avi Swartz are working on this project. No individual roles have been delegated to this point, though Avi seems to have an affinity for deleting existing code (which was totally an accident).

**Current Progress**:

At the moment, we have an existing class hierarchy including space classes such as point and vector, mathematical classes such as matrix, and classed for various atoms which will be used for the folding model. We had a system for 3D rendering model, which had to be scrapped, and we are developing a method of rendering through Sketchup. We have fully implemented the Matrix class with multiplicative methods and rotational methods for instantiating and modifying atoms in three dimensions. We’ve also included a table including the Van der Waal radii of the essential atoms used in the model.

**Current Roadblocks:**

So far, we have encountered many obstacles, including extremely difficult 3D rendering systems. In the future, we will have to work out the incredibly complicated math behind actually folding the protein. Currently, we are tacking the problem of rendering our work, and we have progressed fairly well to achieve this goal. Other than that, we have a fair amount of code that works just fine but doesn’t actually do anything. Until we work out the bigger problems such as the math and a visual representation, our existing infrastructure will not be put to any functional use.

**Future Plans:**

For the future of our project, we plan to first implement the rendering system. We hope to accomplish this task by the date this paper is due. Next, we plan to accept an input in the format of an amino acid chain in its proper primary structure. We also hope to properly “fold” the amino acid chain into its secondary structure. Both of these goals should be accomplished by 1 week after the project is due. In the next two weeks. We will attempt to derive the tertiary structure of an amino acid chain within the next two-three weeks, however this is a very ambitious goal as tertiary structure is the primary focus of our program. To achieve all of our goals, we will all try to work together to accomplish the objectives rather than dividing and trying to individually meet them.

**General Recommendations:**

For general recommendations, we would like to tell any future programmers to comment well and make use of javadocs. Using applications such as GitHub or Dropbox is a good way of granting everyone access to work. Our group uses Dropbox for syncing because we use libraries that require different native files for Mac and Windows operating systems, so using Dropbox we can more easily overcome having to manually change the settings every time. Finally, we would not recommend anyone else (or even us) to try a project like this.