CER Technology Fellowship Program –2008

Project Team: Jeffrey Gray, Assistant Professor, Chemical and Biomolecular Engineering Whiting School of Engineering; Julian Rosenberg, Undergraduate Student, Chemical and Biomolecular Engineering Whiting School of Engineering; Sidhartha Chaudhury, Graduate Student, Biophysics, Krieger School of Arts and Sciences

Project Title: Computational Instructional Modules for Protein Structure Prediction and Design

Audience: Students in the course *Computational and Experimental Design of Biomolecules (540.460)*

Pedagogical Issue: Protein design is a growing area of the synthetic biology field with enormous impact in designing therapeutics, creating novel means of interrogating biology, and creating nanobiological devices. Although a number of programs exist to predict protein structure or design function, most involve little or no interaction from the user and consequently have limited potential in illustrating their underlying principles. Creating a set of hands-on modules would enable students to use state-of-the-art protein simulation software for protein structure and energetics calculations and for protein design. The goal is for students completing the course to be able to efficiently engineer proteins computationally.

Solution: The proposed project will create student access to the protein prediction software (Rosetta) via the creation of tutorials, homework exercises, and a project assignment. The project will leverage efforts in the research community, where the Rosetta protein structure prediction program is being re-written to be readily accessible from the common scripting language, Python. This approach is new and unique because this will be the first time undergraduates will have direct access to the Rosetta program or for that matter any protein structure prediction and design software

Technologies Used: Python, C++, Rosetta

Project Abstract: We will create a set of instructional modules employing the Rosetta protein structure modeling suite to teach applications in protein structure prediction and design. These modules will consist of instructional tutorials, homework assignments and project assignments on computational protein structure prediction and design. Pedagogically, the project will involve students in active and deep learning about the computational protein design process and give them real experience with state-of-the-art software. Students will use the Python scripting language to visualize and manipulate Rosetta objects such as a protein conformation, amino acid sequence, energy functions, and conformational search strategies in order to gain intuition into both the practical and scientific challenges that underlie computational protein design. In order to teach these processes, it is necessary to develop appropriate educational materials for interacting with the complex software. The Fellows will create material to make the powerful capabilities of the Rosetta software available to undergraduates by writing clear tutorials and supporting scripts and necessary supporting objects. The Fellows will also test the software and write appropriate interfaces (in Python and/or C++) where they are lacking. The Fellows are two undergraduate Chemical & Biomolecular Engineering students who have taken a protein design class

and have some programming background; they will work with a graduate student in the Program in Computational and Molecular Biophysics. The modules will be developed and applied to the spring semester course, *Computational & Experimental Design of Biomolecules (540.460)*, assessed with surveys and student performance measures, and made publicly available for use at other institutions.