Modeling proteins with bioinformatics and biophysics

This course will cover modern computational tools to study the annotation, structure, dynamic, and function of proteins, which are the prime machines of the cell. No prior classes on proteins or biology are required but experience in computer programming and physical chemistry (statistical mechanics) is desired.

The course starts with a brief review of what proteins are all about, and continues with the annotation of new unclassified sequences with bioinformatics tools. Tools that will be discussed in detail include sequence comparison, significance of a match, fold recognition algorithms, and three dimensional model building. Emphasis will be made on the design of machine learning algorithms for modeling protein structures. Further exploitation of protein structures will address questions about protein design, sequence evolution, and evolution of protein structures. Finally, computational biophysics models will be used to address questions on protein stability and activity. We shall discuss conformational transitions, ion migration through channels, and kinetics of protein folding. Coarse grained and atomically detailed models will be introduced, illustrated, and used in the class.