Stability of proteins and viscosity of active colloids
Dr. Luis E. Sanchez-Diaz

Understanding the function of biomolecules in terms of their structure is one of the grand challenges for science in the 21st century. It holds the key to a wide range of applications, from biotechnology to pharmacology and medicine. Would you like to learn some computational and experimental techniques to study biological systems? In these systems, macromolecules are constantly moving around by a process called diffusion. How do the molecules find their binding partners? How do they fold to form a particular shape? How do they diffuse through the crowded environment of the cell interior? Biological molecules may exhibit different kinetic and thermodynamic properties under different conditions. My research focuses on understanding diffusion and viscosity of these systems. I invoke concepts from fluid mechanics, statistical physics, and molecular biophysics to develop mathematical and computational tools to learn about the complex hydrodynamic and biochemical processes occurring inside of living systems

This summer we will working on two projects. The first, will be about understanding the stability of proteins using computer simulations (Figure 1). We will begin by learning the basic simulation methodologies and review concepts from statistical mechanics to understand the interactions and behavior of biological systems. Then, we will perform Molecular dynamics to simulate a biological system using a simple model of interaction. We will calculate structural properties like Radius of gyration, RMSD, Radial distribution function and compare with theoretical, computational and experimental results. The second project is to study the rheological properties of a solution of active colloids by using analytical theory and computer simulations. To study this system, we will perform Brownian dynamics to simulate a colloidal system using a simple model of interaction (Figure 2). You will learn about the different properties that can be used to describe diffusion in this kind of system, such as mean square displacement, van hove function, and self-diffusion coefficient, and viscosity. You will be introduced to how scientists can compare simulated results like the ones you have created to theory and experiments.

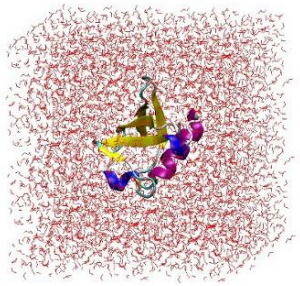

Figure 1

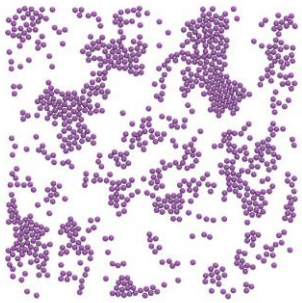

Figure 2

Also, during the summer, we will arrange a visit Oak Ridge National Laboratory. Here you will perform some experiments using an instrument called rheometer, this instrument is used to measure viscosity as function of the force applied. You will also observe the procedure to perform an experiment using neutron scattering. After completing this summer research project, you will be encouraged to present your work at an upcoming regional or national conference.

Students in biophysics with experience in research can pursue jobs in research institutes or industry. For example, biophysicists at the National Institutes of Health in Bethesda, Maryland, study the molecular and cellular basis of disease. Others work at National Laboratories such as in Brookhaven, New York, in Argonne, Illinois, in Los Alamos, New Mexico, or in nearby Oak Ridge, Tennessee.