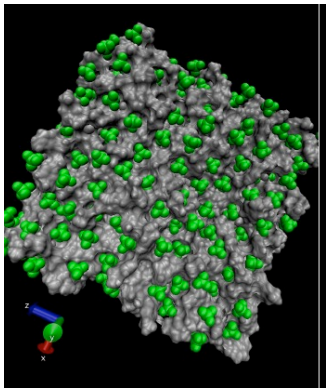
Simulation of colloidal and biological systems.
Dr. Luis E. Sanchez-Diaz

.
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 the 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 an active cell.



Project 1: Molecular simulations of ionic liquids

With the aim to validate the recent predictions of the self-consistent generalized Langevin equation theory, describing the existence of unusual partially arrested states in the context of ionic liquids. Here propose to run molecular simulations of different ionic liquids to calculate the conductivity and compare them with the theoretical framework. Simulations will be performed using GROMACS. Simulations need to run with many particles and longer periods to obtain good statistics. To perform this massive simulation will require the use of the UTC SIMCENTER computer cluster.

Project 2: Brownian dynamics of a mixture of silica particles with lysozyme. Comparison with Rheo-SANS(Small Angle Neutron Scattering) experiments.

Rheo-SANS experiments with a solution of silica particles and lysozyme will be performed at ORNL in spring. Our main goal is to develop a model to compare with the experiments. We propose a simple model for the Brownian motion of colloidal particles and lysozyme under shear steady flow. Previous experiments show that silica particles become sticky when lysozyme is added. In our simulation, the interaction between the silica particles and lysozyme will be described using sticky potential. The code will be built in Python or Fortran. Properties such as structure, shear stress, shear viscosity, and shear modules can be obtained from simulation and compare quantitative and qualitative with experimental results from rheometer.