Background

My research experience is in; percolation theory, transport in disordered media, simulation of diffusion limited aggregates, spinodal decomposition in quenched binary-component fluids, fluctuation driven long-time (material) domain growth dynamics, dynamical chaos, cellular automata models for fluids at low Reynolds numbers, mechanical stability in polymeric and amorphous chalcogenide glasses, generic rigidity theory, graph-rigidity algorithms, protein flexibility, stability and dynamics, allosteric mechanisms and conformational pathways within proteins, structural bioinformatics applications that involve comparative studies across protein families, and solution thermodynamics.

Research Interests

My research interests span statistical and computational physics that is invariably connected to novel algorithm development. My broad interests attract me to interdisciplinary research where there is a need to construct tractable models that balance accuracy and computational efficiency for specific applications. Although I do not perform experiments in a laboratory, I work directly with experimental data to design empirical models, and assess how well the calculations or simulation results compared to observations. I prefer to work closely with collaborators performing the experiments.

Since 1997 my research migrated from condensed matter physics to biophysics, which was the time I decided to apply rigidity theory to study mechanical stability of proteins. Since then, I have developed an awe for the complexity of biological systems, and specifically I have been inspired to take up the open challenge of predicting protein thermodynamics, flexibility and dynamics at a pragmatic level useful for drug discovery workflows. As such, I have continued to investigate these fundamental properties and their interrelationships and have devoted much time to build novel models involving out of the box thinking that do precisely that. In addition, I expanded my investigations to include long-range electrostatic interactions since 2006, and since 2004 I have been interested in the comparative analysis of quantitative stability/flexibility relationships between proteins in order to better understand the physicochemical mechanisms (or constraints) on evolutionary dynamics.

Unfortunately, to date, there does not exist any computational model that meets the grand challenge of drug discovery. However, over the years of making many installments to model development, my research group has consistently made advances each year toward meeting the grand challenge of drug discovery. Although faced with many difficulties, this is a very exciting endeavor!