COLLEGE OF ENGINEERING, COMPUTER SCIENCE, & TECHNOLOGY

Seminar in Interdisciplinary STEM Research

March 27 – Thursday, 3:05-4:20 PM PST

Location: E&T A-256

HOSTED BY CREST-CATSUS AND SIKAND SITI CENTERS

Dr. Negin Forouzesh

Assistant Professor in the Department of Computer Science at California State University, Los Angeles

Dr. Negin Forouzesh is an Assistant Professor in the Department of Computer Science. She earned her Ph.D. from Virginia Tech and completed an internship program at the Stanford Center for Genomics and Personalized Medicine (SCGPM). Dr. Forouzesh is interested in teaching and research in computational sciences with applications in drug discovery. She is the director of the Computational Molecular Biology (COMB) Lab at Cal State LA which develops machine learning models, scalable optimization algorithms, and high-performance computing techniques to understand the structure and function of biomolecular systems.

Physics-guided Machine Learning for Drug Discovery

Abstract: Drug discovery is one of the most complex and time-consuming challenges in biological sciences, typically requiring 10-15 years and an investment of around $2 billion to bring a new drug to market. The primary objective is to identify drug-like compounds, or ligands, that can effectively modulate specific biological targets, usually proteins. A crucial aspect of protein-ligand interactions is the change in binding free energy (ΔG) that occurs when a ligand binds to a protein, which plays a key role in determining the strength of their interaction. Understanding this interaction is essential for drug design. While wet-lab experiments can accurately estimate ΔG, they are often slow, expensive, and labor-intensive. In contrast, computational simulations provide a much faster and more cost-effective way to estimate ΔG, while also offering insights into the binding mechanisms of various structural complexes that might be difficult to study experimentally. My research aims to bridge the gap between physics-based models and experimental data for ΔG calculations by employing modern machine learning techniques. In this presentation, I will share results from my recent and ongoing work, focusing on physics-guided neural networks, deep generative models for novel ligand discovery, and interactive molecular docking in virtual reality.

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