2023 Computational Structural Bioinformatics Workshop

Sunday, September 3, 2023
Workshop Co-chairs: Fardina F Alam, Gideon Gogovi
Each talk is 20 minutes (approximately 15-16 minutes for the talk and 4-5 minutes for Q&A).

8:50-9:00	WORKSHOP WELCOME REMARKS Workshop Co-chairs: Fardina F Alam & Gideon Gogovi
9:00-10:00 AM	KEYNOTE ADDRESS Title: What is the protein electrostatic potential in solution? Speaker: Montgomery Pettitt, University of Texas Medical Branch
10:00-10:15 AM	BREAK
SESSION 1	Protein Structure, Predictions and Bindings
10:20-10:40 AM	Leveraging Large Language Models for Predicting Microbial Virulence from Protein Structure and Sequence. Felix Quintana, Todd Treangen and Lydia Kavraki.
10:40-11:00 AM	Assessing Fairness of AlphaFold2 Prediction of Protein 3D Structures. Usman Abbas, Jin Chen and Qing Shao.
11:00-11:20 AM	AlphaFold2 Model Refinement Using Structure Decoys. Maytha Alshammari, Jing He and Willy Wriggers.
11:20-11:40 AM	Structure- and Energy-based Analysis of Small Molecule Ligand Binding to Nuclear Steroid Hormone Receptors. Megan Herceg and Amarda Shehu.
11:40 AM - 1:00 PM	BREAK
SESSION 2	Cryo-EM, Structural Modeling and Mutation
1:00-1:20 PM	A Containerization Framework for Bioinformatics Software to Advance Scalability, Portability, and Maintainability. Justin Tam, Alexandra Chua, Adyn Gallagher, Denice Omene, Danielle Okun, Dominic DiFranzo and Brian Chen.
1:20-1:40 PM	An Approach to Developing Benchmark Datasets for Protein Secondary Structure Segmentation from Cryo-EM Density Maps. Thu Nguyen, Yongcheng Mu, Jiangwen Sun and Jing He.
1:40-2:00 PM	A Comparative Analysis of Transformer-based Protein Language Models for Remote Homology Prediction. Anowarul Kabir, Asher Moldwin and Amarda Shehu.

2:00-2:20 PM	Identifying Impactful Pairs of Insertion Mutations in Proteins. Changrui Li and Filip Jagodzinski.
2:20-2:30 PM	BREAK
2:30-3:00 PM	PANEL: Navigating Career Path in Computational Biology and Bioinformatics: Overcoming Barriers and Embracing Transformations. Panelists: - Brian Chen, Lehigh University - Filip Jagodzinski, Western Washington University - Negin Forouzesh, California State University, Los Angeles
SESSION 3	Machine Learning/Deep Learning-Based Approaches
3:00-3:20 PM	A Sequence-Based Prediction Model of Vesicular Transport Proteins Using Ensemble Deep Learning. Nguyen Quoc Khanh Le and Quang Hien Kha.
3:20-3:40 PM	RoseNet: Predicting Energy Metrics of Double InDel Mutants Using Deep Learning. Sarah Coffland, Katie Christensen, Filip Jagodzinski and Brian Hutchinson.
3:40-4:00 PM	Optimizing K-Mer Fingerprint Generation for Machine Learning. Cory Kromer-Edwards.
4:00-4:20 PM	Physics-Guided Deep Generative Model for New Ligand Discovery. Dikshant Sagar, Ali Risheh, Nida Sheikh and Negin Forouzesh.
4:20-4:25PM	Closing Remarks

Keynote Lecture/Address:

Speaker: Professor Montgomery Pettitt, Director, Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch

Title and Abstract: What is the protein electrostatic potential in solution?

Molecular mechanics models usually take electrostatic components from scaled quantum chemical calculations and make heuristic adjustments. We wish to check these numbers against experiment. Paramagnetic resonance enhancement NMR experiments (PRE) can measure the electrostatic component of the potential of mean force in solution with spin-probe cosolutes. We compare the experimental PRE results with theory and multi scale simulations to determine the contribution of different chemical components to the near-surface electrostatic potentials in different salt solutions. Salt-dependence of the electrostatic potentials for the protein ubiquitin was studied in ionic strengths from 0 mM to 730mM. The results of Poisson-Boltzmann continuum solvent theory are in good agreement for many of the residues. We found discrepancies are caused by correlations of the probe molecule with the protein in the calculations and are accounted for with multi scale simulations. Mutual validations of the experiment and the computations emphasize the importance of orientational correlations of probes in the determination of surface potentials by PRE. This technique coupling experiment and theory gives a rigorous method to measure molecular electric fields.

Time: 9:00-10:00 AM (CST)

Bio:
B. Montgomery Pettitt is the Robert A. Welch Distinguished University Professor of Chemistry, and director of the Sealy Center for Structural Biology and Molecular Biophysics. He is a faculty member of Pharmacology and Toxicology and is both professor and interim chair of Biochemistry and Molecular Biology. He organized and currently leads the research biomedical informatics program for the CTSA at UTMB. He came to UTMB in 2012 from the University of Houston where he had been chair of Chemistry, Computer Science, as well as Associate Dean of Computational Science and Associate Dean for Research. His research applies theoretical chemistry to solve computational problems in molecular biophysics.