Session H Abstracts

Episomal DNA isolation for oncogenic virus detection and viral vector discovery
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Mentors: Rustem F. Ismagilov, Christopher Neimeth, and Natalie Wu-Woods

Abstract withheld from publication at mentor's request.

Lower time complexity of DNA winner take all neural network combining shared fuel amplification and pairwise annihilation
Anthony K. Lindo
Mentors: Lulu Qian and Matthew Plazola

DNA's ability to participate in toe-hold mediated displacement reactions allows the molecule to be programmable and participate in a numerous amount of computer science principles. One of the most promising are DNA neural networks. There are two implementations of a winner take all behavior known as pairwise annihilation and shared fuel amplification. Pairwise annihilation involves weighted sums eliminating each other until there's a single survivor and then later restoring itself to produce a signal of 1 while the losers remain 0. The advantage associated with this system allows it to be robust to changing strand concentrations while the disadvantage is it's O(n^2) time complexity with each increasing input. Shared fuel amplification involves a host of weighted sums competing for a shared fuel strand while surviving sequestration from thresholding strands. The advantage associated with this system allows it to occur at an almost linear time complexity, but it's much less robust and doesn't exhibit true winner take all. The winning strand doesn't compute to 1 but a steady state that requires a look up table. I'm developing a system that allows the system to remain robust while maintaining a linear time complexity. By allowing a fuel strand to remain competitive throughout the system and letting the threshold get the winner to near 0, and having restoration occur afterwards, the winning strand can compute to 1 much quicker than having it compete with other losing strands directly.

On the computational power of nucleation kinetics
Ritali Jain
Mentors: Erik Winfree, Cameron Chalk, and Yancheng Du

Self-assembly is a prevalent molecular phenomenon in the chemical world—from the formation of viral capsids to crystalline structures—with ties to algorithmic behavior arising from programmable local interactions. One particularly interesting kinetic regime is nucleation, a rare event process whose dynamics involve stochastic exploration to overcome an energy barrier and eventually stabilize into an energetically favorable structure. It has been demonstrated that self-assembly under nonequilibrium nucleation kinetics can be programmed to form structures classifying high-dimensional concentration patterns, analogous to neural network-like pattern recognition capabilities. While the previous system responded to given input concentrations by colocalizing particular preferred critical nuclei, in this work, we extend this exploration beyond behaviors reminiscent of associative recall to ask whether nucleation kinetics can support richer forms of computation—specifically, the ability to solve constraint satisfaction problems representative of NP-hard search. To investigate this, we encode constraints of NP-hard problems into DNA-based tile components, coupled with the energetics of tile entropy and bond cooperativity. We formally connect the set of tiles' low-energy configurations to low-barrier growth trajectories, lifting an equilibrium constraint satisfaction problem into nucleation kinetics. Since kinetic behavior is also controlled by the entropic distribution of trajectories, we simulate our tiling systems with forward flux sampling and empirically validate that nucleation kinetics performs combinatorial search by a difference in nucleation rates. Although our constructions illustrate the computational power of nucleation in principle, the tradeoff with nucleation speed is significant, and worst-case behaviors remain slow. Nonetheless, this work lays the theoretical foundation for understanding nucleation kinetics as a medium for constrained combinatorial search and empirically supports the role of energy landscape design in shaping assembly dynamics, at least in the context of nucleation.

Interpretable deep learning for functional fine-mapping of chromatin QTLs in Alzheimer’s Disease
Clara Yu
Mentors: David Knowles and Shinsuke Shimojo

Chromatin quantitative trait loci (caQTLs) link genetic variation to changes in chromatin accessibility and transcription factor (TF) binding, offering insight into the regulatory basis of disease risk. This project aims to develop an interpretable deep learning pipeline to fine-map caQTL variants in Alzheimer’s Disease by identifying disrupted TF binding motifs across relevant cell types. Using pre-trained ChromBPNet models, base-pair resolution attributions were generated for caQTL variants in microglia, applying DeepLIFT/SHAP to quantify sequence contributions. These attributions were integrated with Tangermeme for motif discovery and annotation using the HOCOMOCO v11 and JASPAR databases. Variant-level analyses revealed that 60.8% of variant-fold pairs showed motif changes, with agreement between predicted motifs and ChromBPNet consensus TFs increasing from 2.6% to 53.7% when grouping motifs by families. These results highlight the value of motif family aggregation for capturing shared TF sequence preferences. Future work will extend this pipeline to additional brain cell types (neurons, astrocytes, oligodendrocytes) and refine TF annotations by reconciling discrepancies between model-predicted motifs and consensus TFs. This approach demonstrates how interpretable deep learning can bridge variant-level predictions and regulatory mechanisms, advancing our ability to pinpoint functional loci underlying disease-associated noncoding variation.

Unsteady inertial effects in cardiovascular flows: Experimental observations and analysis
Malia A. Christy
Mentors: Michael Plesniak, John O. Dabiri, and Kartik Bulusu

Cardiovascular diseases linked to carotid artery dysfunction remain a significant global health concern, with wall shear stress playing a critical role in atherosclerotic plaque formation. Understanding the hemodynamics that give rise to such stresses requires accurate modeling of unsteady pulsatile flow in arterial geometries. We investigated inertial effects in a 180-degree curved artery model under physiological flow conditions using the dimensionless Womersley number to characterize the influence of pulsatile flow. Due to the multi-harmonic nature of blood flow, a range of Womersley number is expected, which may introduce distortions in experimental measurements and complicate correlations with human vascular flow conditions. Utilizing a custom-built flow loop with a programmable pump, pressure transducers and flow rate sensors, we use water as a Newtonian blood analog to simulate arterial flow. The system was designed using dynamic similarity principles and analytical solutions to the unsteady Navier-Stokes equations. Through combined measurements of pressure gradients, flow rates and wall shear-stress, this work enables more accurate replication and analysis of complex cardiovascular flow environments.

Wake dynamics and propulsive efficiency of natural and biohybrid robotic jellyfish
Kyra T. Phaychanpheng
Mentors: John O. Dabiri and Simon Anuszczyk

The ever-changing nature of our oceans demands innovative methods to better understand and monitor their conditions, ecosystems, and dynamics. However, current ocean monitoring tools face the common challenge of propulsive efficiency as a limiting factor, and are limited to fully mechanical underwater autonomous vehicles or purely biological approaches. A biohybrid robot jellyfish—a live *Aurelia aurita* equipped with engineered electronics that electrically stimulates the jellyfish to contract—combines biological efficiency with programmable control. We investigated and compared the wake dynamics of naturally swimming and biohybrid *Aurelia,* the latter being electrically stimulated to pulse at regular two-second intervals. Yet, understanding how engineered stimulation alters their natural propulsion is key to evaluating their efficacy as biohybrid systems. To analyze this, a 3D Particle Image Velocimetry (PIV) scanning system was employed, in which laser sheets repeatedly scanned over the tank to illuminate the pulsing jellyfish and the subsequent motion of suspended micron-size particles in the water. Animal swimming dynamics were captured by a high-speed camera. A custom MATLAB program then identified and reconstructed the 3D volume for each time step and performs the PIV. With this, we constructed velocity vector fields from the data and calculated vorticity in 2D and 3D with original MATLAB scripts. These metrics allow for a comprehensive analysis and modeling of the jellyfish's kinetic energy, wake dynamics and structure evolution. This research not only advances our understanding of jellyfish locomotion and energetics, but moreover, their downstream capability. In future applications, biohybrid jellyfish may serve as live, low metabolic cost and high efficiency sensors capable of detecting climate changes, monitoring ocean conditions, and exploring deep-sea environments.