Session O - Computation and Neural Systems/Civil Engineering/Environmental Science and Engineering
(Alphabetical)

A Kinetics-Optimizing DNA Sequence Designer
Christopher G. Berlind
Mentor: Erik Winfree and Joseph Schaeffer

Experiments in the realm of DNA nanotechnology are often heavily dependent on the kinetics of the reactions involved, which in turn are determined by the nucleotide sequences of the interacting DNA strands. While this observation suggests that kinetic data can be used as a good measure of the quality of a particular DNA sequence, methods of computational sequence design to date have not focused on kinetics. Instead, design methods have been based on combinations of criteria such as sequence symmetry, thermodynamic stability, and ad hoc criteria. These design criteria have varying levels of correlation with kinetic data, and some have been observed to be very poor predictors of kinetics. In an effort to take advantage of better design criteria, we present a DNA sequence designer that optimizes sequences for kinetics primarily through the use of stochastic kinetics simulations. We explore the efficiency of several optimization methods including stochastic hillclimbing, nested partitioning, evolutionary algorithms, and combinations thereof. We then compare the efficiency of our kinetics-based designer with those of other sequence designers, analyzing the quality of designed sequences using simulations.

Effect of Value of a Visual Stimulus on its Preferential Access to Awareness
Laura H. Conwill
Mentors: Christof Koch, Milica Milosavljevic

Our visual system is constantly exposed to a cluttered environment. Due to our limited processing capacity, navigating such an environment requires giving preferential access to objects of importance. It is known that we give preferential access to objects that elicit an emotional reaction. Here, we investigated how the subjective values of objects affect their access to awareness. We used the method of continuous flash suppression to examine whether the subjective value of an item (how much a person likes that item) affects its access to awareness (how quickly the item is perceived).

Development of Electrochemical System for Simultaneous Hydrogen Production and Degradation of Real Wastewater
Ning Du
Mentors: Michael R. Hoffmann and Jina Choi

Conventional electrochemical water splitting produces molecular hydrogen at the cathode, while oxidation takes place at the anode. An electrolytic cell based on bismuth-doped TiO_2 anode and stainless steel (SS) cathodes is used in the experiment to characterize the efficiency of organic waste degradation and hydrogen production in different wastewater sources: landfill groundwater, river surface water, and manufacturing organic wastewater. For each source, chemical oxygen demand (COD) is measured as parameters indicating organic contents before, during and after each electrolysis experiment. Various operating conditions including DC power voltage, pH, conductive electrolyte type and time of electrolysis are investigated to optimize wastewater degradation. Results show that for manufacturing organic wastewater, significant amount of organic content is degraded within 2 hours under all operating conditions. On the hydrogen production side, gas chromatography (GC) is used to analyze hydrogen content during electrolysis of salt water employing electrodes consisting of SS cathodes and various metal-doped TiO_2 anodes. Results show Pt-, Ru-, Cu- and V-doped anodes to generate hydrogen within 30 minutes. Both parts of the experiment aim to construct a high performance electrochemical system for practical use in industrial and municipal wastewater treatment.

The Upper Ocean Fresh Water Content in the Nordic Seas
Sarvesh Garimella
Mentor: Daniela Di Iorio

The Nordic Seas incur changes in water density during the Northern Hemisphere's winter that correlate to changes in water salinity. We compare observed salinity anomalies with existing heat content measurements to quantify and compute freshwater content in the Nordic Seas and show the seasonal and interannual variability. In order to survey the freshwater content of these basins, we analyze Argo float data collected between 2001 and 2009. Concentrating on the data from the Greenland Sea (GLS) and Norwegian Sea (NWS), we determine both the anomalous heat and freshwater contents (AHC and AFC) for each basin over time with reference to regional 2005 World Ocean Atlas climatological standards. Our observations indicate that AHC is increasing in the GLS and that it is decreasing in the NWS, where there is also more inter-annual variability. They also indicate that AFC is increasing in the GLS while the NWS still shows significant inter-annual variability. Finally we see that the AHC and AFC are strongly correlated within both basins: GLS AHC and AFC have a correlation coefficient of 0.50 and NWS AHC and AFC have a correlation coefficient of 0.83, which indicates that increases in heat correlate to increases in freshwater in both basins.

Test and Optimization of Spike Sorting Algorithms through Biophysical Modeling
Fan Huang
Mentors: Christof Koch and Costas Anastassiou

Spike sorting, the process of determining the extracellular signature of each neuron based on the location of each recording cite, is the cornerstone for experimental investigations of neural rate and phase encoding. A major difficulty in spike sorting is that neither the optimal features for distinguishing spike classes in a given data set nor the number of spike classes needed to completely describe a given data set can be known a priori. Herein, we examine existing spike sorting algorithms using models of neuronal population emulating the experimentally measured extracellular activity where the source neuron of each spike is known. We first characterize and test the efficiency of four spike sorting algorithms using spiking-neuron models at various abstraction levels, from the simple ball-and-stick model of the neuron to population models of anatomically and functionally realistic neurons. In addition, we develop clustering procedures so as to optimize for a specific target of interest, such as determining the most efficient strategy to measure the signal from cells further away from the implanted wire. This research could lead to the suggestion of more efficient sensor architectures and alternatives for tetrodes.

Autonomous Navigation of a Montgolfier Within Micro-Climates on Titan
Robert F. Karol
Mentor: Jerrold E. Marsden

Ever since the Huygens probe pierced through Titan's atmosphere revealing lakes of methane and an atmospheric composition very similar to that of Earth, a second mission has been in the making. The current proposal for this new mission involves deploying a hot air balloon and taking measurements while it floats through Titan's atmosphere, which is perfect for such aircraft. However, little is known about Titan's winds. Of specific interest to this project is how to navigate a hot air balloon by altitude adjustments without prior knowledge of the winds. Terrestrial hot air balloon pilots gave insight into the techniques they use during ballooning competitions which may be applicable to a balloon on Titan. GPS data was then gathered from a variety of pilots flying towards a common goal. From this data and the geographic features of the area, a general idea of the wind currents that day, and possible causes of such currents could be determined. Comparing the data to the model of the day's wind currents can help determine the accuracy of such models.

Modulation of Neuronal Responses by Stimulus Category and Attention Across the Medial Temporal Lobe
Simon Kornblith
Mentors: Christof Koch and *Florian Mormann*

While lesion studies have shown that the medial temporal lobe (MTL) serves a fundamental role in memory storage and maintenance, very little is known regarding the roles of individual MTL subregions. Analysis of data acquired from single neuron recordings in human patients indicated that the amygdala and parahippocampal cortex roles are specialized for processing animal and spatial stimuli, respectively. In both of these regions, analysis of the proportion of selective single neuron responses across a large population of patients indicated a significant category preference. Local field potentials (LFPs) in the parahippocampal cortex were also selective for spatial stimuli, with the onset of LFP selectivity significantly preceding the spiking response. The results of an investigation of the effect of attention upon single neuron responses during a rapid serial visual presentation (RSVP) paradigm will also be presented.

Control of Biological Noise in Molecular Automata
Gabriel Mendoza
Mentor: Yaakov Benenson

Molecular automata show promise to diagnose and treat human diseases at the cellular level. However, the stochastic nature of cellular processes will present a challenge for the reliable operation of such devices. In this research, we designed and implemented molecular network motifs to control variation in gene expression output. The design process involved exhaustive combinatorial simulation of 2 and 3 node networks, and the identification of low-noise promoters based on experimental data. We hypothesize that forthcoming results will confirm the noise-reducing properties of the network motifs.

Seesaw Gates in RNA
Amy Proctor
Mentors: Erik Winfree and Lulu Qian

Organisms use complex biochemical circuits to process information and control tasks essential for survival and reproduction. Synthetic biology applies engineering principles to the biological sciences to design and fabricate analogs to cellular regulatory networks to probe molecular behavior and to harness biology as a means of influencing information, materials, and energy. Of specific interest for this project are nucleic acid systems that exploit predictable Watson-Crick base pairing and toehold mediated strand displacement reactions to implement circuits. Previously implemented in DNA, the seesaw gate motif is modular and scalable, making it suitable for the construction of large-scale circuits. Here, we attempt to implement the catalytic seesaw gate architecture in RNA.

Leak Suppression for Catalyzed Nucleic Acid Entropy-Driven Reactions
Karthik Sarma
Mentors: Erik Winfree and David Yu Zhang

Nucleic acids provide a useful mechanism for constructing molecular-scale computing elements because the predictable nature of Watson-Crick hybridization allows for rational sequence design and because the combinatorial sequence space allows for the encoding of many different signals. Molecular-scale computing elements have potential applications in nanoengineering, targeted pharmaceuticals, and chemical engineering. In particular, nucleic acid amplification mechanisms are needed in order to process very weak signals (which correspond to molecules in low concentration, such as mRNA transcripts in a cell). Ideal amplification mechanisms produce a large quantity of output in the presence of their signal and produce little to no output in its absence. The effectiveness of catalytic amplifiers can be measured by their catalytic efficiency, which is measured as the ratio of their catalytic rate to the uncatalyzed rate. We are investigating a system in which the uncatalyzed rate has been suppressed by 1-2 orders of magnitude relative to a previous system. Unfortunately, this new system currently suffers from a decreased catalytic rate, yielding no overall improvement in the effectiveness metric. We are currently investigating mechanisms by which the catalyzed rate can be increased and the uncatalyzed rate further suppressed in order to increase the effectiveness of our amplifier.

Steel Building Collapse Analysis: Closer Look at the Blind Analysis Contest of a Four-Story Building
Sang Ha Shin
Mentor: Swaminathan Krishnan

Predicting the behavior of steel structures under the influence of earthquakes is difficult. FRAME3D is a program that aims at achieving this goal. Using FRAME3D, Professor Krishnan participated in a blind analysis contest in which he predicted the collapse behavior of a four-story building. Most of the data that he submitted did not match the actual behavior except the collapse time of the structure. This research is to find out more about why this happened. Understanding how to run the program and analyzing the output is the key.

A Verifying Compiler for DNA Chemical Reaction Networks
Seung Woo Shin
Mentor: Erik Winfree

Recently, many different methods have been proposed to implement a given chemical reaction network with DNA molecules. Chemical reaction networks then become a powerful programming language for DNA computing since they are known to emulate the Turing-universal register machine with an arbitrarily small probability of error. Also, chemical reaction networks are a much higher-level programming language than DNA sequences and can greatly reduce the tedious maneuver repetitively carried out in most DNA computing labs. Here we present a compiler that translates a given chemical reaction network to DNA molecules. The compiler is designed to support many different translation schemes by having yet another programming language in which the user can describe them. In addition, the compiler tests whether the compiled DNA molecules behave to the specification. We are also working on a method to prove the general correctness of a given translation scheme. A theoretical basis for realizing those automated proofs is discussed in the paper, and it focuses on the reachability between states in the system. Overall, our compiler will not only provide an essential step toward an even higher-level programming language for DNA computing, but also help facilitate various lab works in relevant fields.

Adapting Non-Nucleic Acid Input to a DNA Circuit

Talia Weiss
Mentors: Erik Winfree and Lulu Qian

The future success of implementing circuitry in DNA highly depends on the “Plug and Play” aspect: that separate components originally intended in one particular function can be easily reworked and plugged into an entirely different circuit. This project tests the validity of this aspect of DNA computing by adapting an ATP aptamer containing hairpin (an “aptasensor”) previously used with a hybridization chain reaction, and having it act as ATP sensing input to a seesaw gate, a general DNA circuit motif that can easily be built up into large scale circuits. By experimenting to learn how to adapt this aptasensor to the seesaw gate motif, one gains insight on what conditions are important to maintain for converting components to work in different DNA systems.