Discrete Mathematical Biology, Part II
(Org: **Torin Greenwood** and/et **Christine Heitsch** (Georgia Institute of Technology))

PETER CLOTE, Boston College
Network properties of RNA secondary structures

The kinetics of RNA secondary structure folding depends on properties of the exponentially large collection of structures. In this talk we describe methods to efficiently compute certain network properties of RNA – for instance, expected degree, as well as new, yet unpublished results.

ELENA DIMITROVA, Clemson University
Unique Reduced Gröbner Bases of Ideals of Points

Computation of vanishing ideals of points comes with challenges even over finite fields. Gröbner bases are the standard tool for computation but for most sets of points the vanishing ideal has several equally "nice" generating sets. These sets yield multiple interpolating polynomials which is not optimal in the context of model selection. In this talk, we will identify properties of the points that result in a unique reduced Gröbner basis for the ideal and see how they benefit the design of experiments and selection of algebraic models of systems in mathematical biology.

TARA PETRIE, Simon Fraser University
Folding something other than laundry

RNA (ribonucleic acid) is the connection between genetic information and proteins. The nucleotides adenine (A), uracil (U), guanine (G), and cytosine (C) are the building blocks of RNA. The nucleotide A pairs with the nucleotide U, and similarly G pairs with C. These nucleotide pairings create folds in the RNA sequence, which we refer to as the secondary structure. The secondary structure's stability increases with the number of pairings, but in general, even with a maximum number of pairings, there is more than one way a sequence of nucleotides can fold. This motivates the *combinatorial RNA design problem*: given a target secondary structure T, can we specify an RNA sequence which can achieve its maximum number of nucleotide pairs in only one way, namely by folding into the specified secondary structure T. This talk examines the case where all nucleotides are paired and the trickier case where some go unpaired.

CHRISTIAN REIDYS, Virginia Institute of Technology
a new grammar for PK-structures

RNAFeatures is a novel grammar, capable of generating any RNA structure, including pseudoknots (PK). PK-structures seen as fat-graphs, lead to a filtration by their genus, with RNA secondary-structures corresponding to PK-structures of genus zero. RNAFeatures acts on formal, arc-labeled RNA secondary-structures, called lambda-structures. These correspond one-to-one to PK-structures together with decorations that consist of backbone permutations, for which the PK-structure is crossing-free. RNAFeatures employs an enhancement labeling of symbols and production rules. RNAFeatures is used to obtain a stochastic context-free grammar for PK-structures, using RNA sequences and structures. The induced grammar facilitates fast Boltzmann sampling and statistical analysis.

DAVID SIVAKOFF, Ohio State University
Discrete Excitable Media

Excitable media are characterized by a local tendency towards synchronization, which can lead to waves of excitement through the system. In discrete models of excitable media, one is interested in whether or not sites are excited infinitely often, and if

so, whether the density of domain walls between disagreeing sites tends to 0. We introduce a new comparison process, which lets us study the asymptotic rate at which a site gets excited in two classical models of excitable media, as well as a novel model for pulse-coupled oscillators introduced by Lyu in 2015. Based on work with Lyu and Gravner.