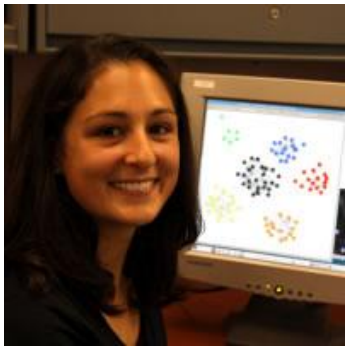
McCormick

Northwestern Engineering

Lectures in Chemical and Biological Engineering

Investigating Folding Dynamics of RNA Through Conformation Space Networks



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Biological polymers, such as RNA and proteins, depend directly on their three-dimensional structure in order to perform properly within the cell. The number of conformations a polymer may adopt is staggeringly large, and the difficulty of predicting folding trajectories grows exponentially with length. To gain insight on the RNA folding problem, we coarse-grain the RNA single strand into the major components of the phosphodiester bonds, the nitrogenous bases, and the sugar groups, and constrain their movements to a lattice. Traditionally, RNA folding has been studied using experimental techniques, molecular dynamics simulations, or Monte Carlo simulations. A complementary approach to understanding the "rules" of RNA folding dynamics is to analyze a conformation space network (CSN). A CSN uses a trajectory of conformations obtained by Monte Carlo simulations to construct a network in which each node is a conformation, and conformations are linked by an edge if an elementary move can transform one conformation into another. Once these networks are generated, we can then calculate various network properties such as the degree and centrality of each conformation and relate these network properties directly to results from high-temperature Monte Carlo simulations. For example, the degree of the conformation indicates how many transformations a conformation can make, while the centrality of the conformation indicates the relative importance of the conformation to the folding pathway. Importantly, these network properties convey relevant information about the folding process with considerably less computational cost.

Thursday October 8th at 4:00PM in Tech LR4
The Technological Institute
2145 Sheridan Road
Refreshments will be served at 3:45 PM