Mathematics Colloquium

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Monday, December 9, 2019
Time: 3:00 p.m.
Location: Weber 223

Title: Mathematical Models of Biomolecules

Abstract: Biomolecules, such as proteins, DNA and RNA, and lipid membranes, are biological building blocks. Their structures and dynamics determine how cells function. Efficient and accurate modeling of biomolecules is, however, extremely challenging due to their enormous complexity. In this talk, I will first present a variational model of biomolecular shapes and show some related computational results. I will then describe a hybrid approach to studying how fast or slow a small molecule (e.g., a drug molecule) binds to and unbinds from a large molecule (e.g., a protein), and how fluctuations of water molecules impact such binding and unbinding processes. This approach is a combination of our variational model, an optimization method for finding optimal paths, and stochastic simulations. I will finally discuss the consequences of our findings and the related mathematical issues for future studies. No knowledge of biomolecules is assumed for this talk.

Host: Yongcheng Zhou

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