Utilizing Computational Methods to Predict Allosteric Networks in Protein Complexes

Dr. Quentin Johnson, Postdoctoral Fellow
National Institute for Mathematical and Biological Synthesis
University of Tennessee, Knoxville, TN

Allostery is a fundamental control mechanism used to regulate many biological processes that range from ligand binding to transcriptional activation. In the context of proteins and protein complexes, allostery is the ability of one binding site to influence another distant site. This means that proteins can self-regulate or be regulated by other macromolecules without the need for proximity. This type of distal signaling is used as the basis for molecular switches, cellular signaling, and oxygen transport. While the importance of allostery is well appreciated, a clear understanding of the process still eludes modern science. This is chiefly due to the fact that the residual networks involved in this process are vast and complex, also the physical interactions that sustain these networks occur on an atomistic level and a picosecond timescale. Therefore, it can be quite vexing to study allostery using traditional methods. Still, the rewards far outweigh the frustrations, as an understanding of allostery can lead to the physical control of molecular switches and downstream cellular responses. Here, I discuss a novel computational approach for the detection of allostery in protein complexes by way of molecular dynamics simulation and advanced data reduction protocols.

Bell Hall 143
Friday, February 5, 2016, 10:30 AM

For more information, please contact the Colloquium Chair, Dr. Chuan “River” Xiao, at cxiao@utep.edu or 915.747.8657.