SIAM/APPLIED AND NUMERICAL ANALYSIS SEMINAR

Date: November 4, 2020

Speaker: Alberto Perez

Title: Making sense of macromolecules: Bayesian inference and Markov Models in Structural Biology

Abstract: We are interested in understanding how proteins and nucleic acids self-assemble and interact with each other through computational modeling. The challenge is the large amount of possible conformations – too many to sample exhaustively. We use computational techniques based on Molecular Dynamics to understand how these macromolecules behave – integrating newton's equations of motion at the femtosecond scale. But, self-assembly and binding happen in timescales that are several orders of magnitude longer. To make them feasible, we use advanced sampling techniques such as Bayesian inference on noisy data.

Ultimately, we get conformational ensembles which with gigabytes of data that have to be rationalized. To do so we use techniques of data reduction like PCA or tICA. Recently we have started using Markov State Models as a way to rationalize the pathways and kinetics in our systems.